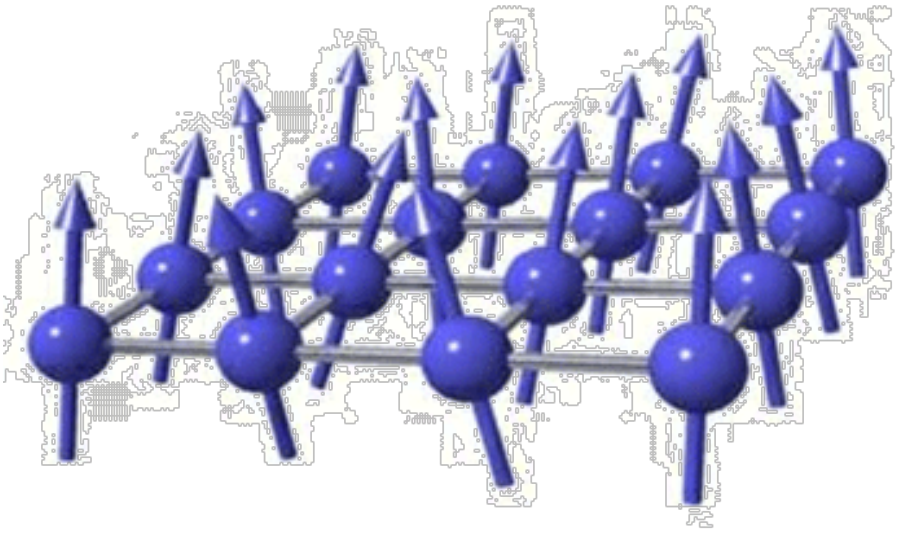


From Quantum Spin Models to Matrix Product States

João Pedro dos Santos Pires
Mestrado em Física (Especialização Teórica)
Departamento de Física e Astronomia
2017

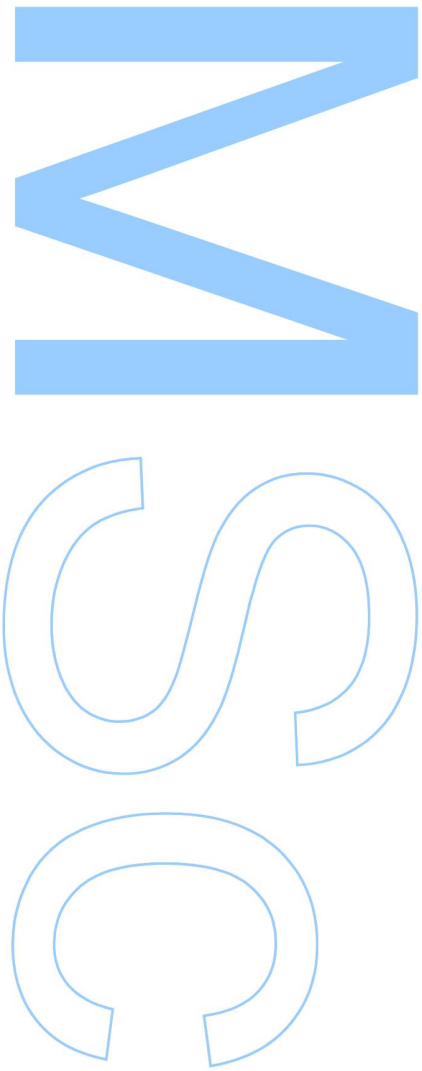
Orientador
João Manuel Borregana Lopes dos Santos, Professor Catedrático, FCUP

Co-orientador
João Manuel Viana Parente Lopes, Professor Auxiliar Convidado, FCUP

Todas as correções determinadas pelo júri, e só essas, foram efetuadas.

O Presidente do Júri,

Porto, _____/_____/_____



From Quantum Spin Models to Matrix Product States

João Pedro dos Santos Pires

Supervisor: Prof.º Dr. João Manuel Borregana Lopes dos Santos

Co-Supervisor: Prof.º João Manuel Viana Parente Lopes

Master's Thesis

Submitted in fulfilment of the requirements

for the degree of Master of Science in the

Departamento de Física e Astronomia
Faculdade de Ciências da Universidade do Porto

Porto, 12^{th} October 2017

"Through the fish-eyed lens of tear stained eyes
I can barely define the shape of this moment in time
And far from flying high in clear blue skies
I'm spiraling down to the hole in the ground, where I hide.

If you negotiate the minefield in the drive
You beat the dogs and cheat the cold electronic eyes
And if you make it past the shotgun in the hall,
Dial the combination,
Open the priesthole,
And if I'm in, I'll tell you what's behind the wall."

Roger Waters, 1983

[This page was intentionally left blank]

Acknowledgments

I wish to thank to all the people who did help, in a greater or lesser degree, during the making of this thesis.

Firstly, I wish to thank my supervisor - Prof. Dr. João Lopes dos Santos - for introducing me to the subject (in particular, by recommending Wen's book and a number of other very interesting pieces of literature) and also for some helpful suggestions and useful discussions at the weekly group meetings. I also thank my co-supervisor - Prof. João Viana Lopes - for the long conversations, his constant availability for helping and also for some useful suggestions.

I also thank my dear colleagues and friends for all the support and cooperation during the last 5 years (or even longer). A particular attention goes to my friends António Leite Antunes and Simão Meneses João, who helped me to clarify some ideas with very interesting and demanding discussions (as usual) and to Maria Pestana Ramos for all the laughs shared at the bar, while we both injected caffeine onto our bodies.

The last, but not the least, I wish to thank my family for all the support, not only during the production of this thesis, but since I embarked in this long and tortuous journey of becoming a physicist.

[This page was intentionally left blank]

Abstract (in English):

In this thesis, we explore several theoretical methods and paths that can be taken for studying the physics of antiferromagnetic quantum spin models. In the first three chapters, the well-known Heisenberg Model is thoroughly explored by using, first, the standard Spin-Wave Theory (Ch.1) and also field-theoretical methods (Ch. 3). These paths allowed us to draw conclusions about the main features of its ground-state and low-energy excitations. In Ch. 2, we prove some rigorous results on the low-energy states of this model and also discuss the concept of magnetic order, proving that it cannot be observed in one- or two-dimensional systems, at finite temperatures.

In the last two chapters, we take account of some interesting one-dimensional antiferromagnetic models whose ground-states can be built exactly. These models are generalized to higher-dimensional lattices and are rigorously proven to be gapped and have a disordered ground-state, in the thermodynamic limit. Finally, these models serve as an inspiration for introducing the concept of Matrix Product States, which is being recognized as an important resource for numerical investigation of strongly-interacting condensed matter systems.

Resumo (em Português):

Nesta tese de mestrado, exploramos diversos métodos teóricos que podem ser usados para estudar a física de modelos antiferromagnéticos de spins quânticos. Nos primeiros três capítulos, o conhecido Modelo de Heisenberg é abundantemente explorado usando, primeiro, a habitual Teoria de Ondas de Spin (Cap. 1), mas também poderosos métodos de Teoria de Campo. Estes tratamentos permitiram-nos retirar conclusões acerca das principais caracteristícas do seu estado fundamental e excitações de baixa energia. No Cap. 2, provamos alguns resultados rigorosos acerca dos estados de baixa energia para este modelo, e ainda discutimos o conceito de ordem magnética, provando que ela não pode ser observada em sistemas uni- ou bi-dimensionais, para nenhuma temperatura finita.

Nos dois últimos capítulos, tomamos em consideração alguns modelos unidimensionais interessantes, cujo estado fundamental pode ser construído exactamente. Estes modelos são generalizados para redes de dimensão mais elevada e é mostrado rigorosamente, que estes modelos têm um 'gap' e um estado fundamental desordenado, no limite termodinâmico. Finalmente, estes modelos servem de inspiração para introduzir o conceito de 'Matrix Product States', que é reconhecido como um recurso importante para a investigação numérica de sistemas de Matéria Condensada, como fortes interações.

[This page was intentionally left blank]

Introduction

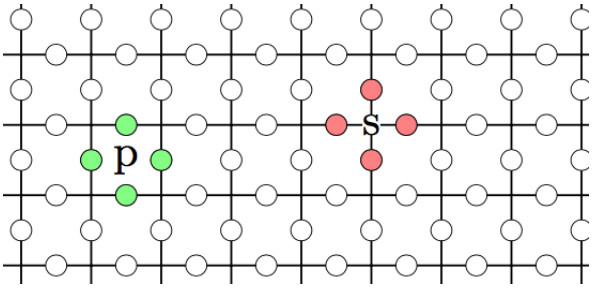
A Personal View

This Master's project began as an attempt to understand the very interesting ideas discussed by Xiao-Gang Wen in his newest book [36], as proposed by my supervisor. In this book, the concept of topological order in condensed matter is discussed, focusing in its connection to Quantum Information Theory and the entanglement properties of some quantum states. These states appear as ground-states of quantum spin models or low-dimensional strongly correlated electronic systems (e.g. the Fractional Quantum Hall Effect), and some examples are discussed throughout the book. From all these examples, one particular system captured my attention - the Kitaev's Toric Code:

This model consists of a square lattice of spins-1/2 (with PBC), interacting through a very special Hamiltonian:

$$H_{Toric} = -U \sum_{s} Q_s - g \sum B_p$$

$$with Q_s = \prod_{j \in star(s)} \sigma_j^z \; and \quad B_p = \prod_{j \in plaquette(p)} \sigma_j^x$$



The Toric Code Model, with the Stars and Plaquettes represented by s and p, respectively.

Despite being a strange looking Hamiltonian, it reveals some striking properties which amazed me from first sight. First of all, its exact ground-state can be built simply by a geometrical construction (called a string-net condensate), but more impressively, its excited states can be proven to be associated to local quasiparticles which behave as fermions interacting via a gauge field. In some sense, it can be said that a theory of light and electrons is an emergence property of this fundamental spin model.

This realization was fascinating for me, but also an utter lesson of humility. In fact, I quickly saw that all the formalism involved in these wild ideas was way above my current level of knowledge. Hence, I decided that I should draw my attention to studying extensively the subject of quantum spin models, with the hope that this knowledge will provide the tools and pave the way to a deeper understanding

of these problems. The present thesis is the, a deep, detailed and pedagogical account of the important theoretical methods and results that I have obtained during this quest.

The Structure of the Text

The text of the thesis is organized logically in five Chapters and an Appendix. An effort was made to keep all of the different Chapters as self-contained as possible, although some calculations may require recapping some results obtained in previous chapters. The Appendix contains some of the lengthy (or boring) calculations needed to justify the results that are being used in the main text.

Thematically, the organization of the thesis is as follows:

- In the **first chapter**, I developed the formalism of spin-wave theory and applied it to the isotropic Heisenberg model (ferro- and antiferromagnetic), calculating the approximate ground-state and low-energy excitations. These results were then used to study energetic and thermodynamic properties of these systems, in several different lattices configurations;
- In the **second chapter**, I explored and defined the concept of magnetic long-range order, culminating in the proof of the well-known Mermin-Wagner Theorem, that rules out magnetic order for one- and two-dimensional systems. Secondly, some important theorems about the Heisenberg AFM models were proved, namely that the ground-state is a singlet of the total spin, and also that the lowest-energy excitations are gapless for all the lattices with half-integer local spins;
- In the **third chapter**, I took a different approach to these problems, making use of more advanced field-theoretical methods. I started by reformulating the model in terms of path-integrals, which eventually led to the Haldane mapping between the Heisenberg Model and the Non-Linear Sigma Model (+ topological terms). Using this mapping, we were able to prove that the integer spin chain is gapped and disordered (Gapped Spin Liquid), which is the celebrated Haldane Conjecture;
- In the **forth chapter**, I studied different spin Hamiltonians, whose exact ground-states can be built. Namely, I have studied the spin-$1/2$ Majumdar-Ghosh model (which includes next-nearest-neighbor interactions) and also the spin-1 AKLT model (which included a biquadratic coupling among first-neighbors, besides the usual Heisenberg interaction). For both models I was able to build the exact ground-states (for finite and infinite chains), check that they only have short-ranged correlations and also prove rigorously that these systems are gapped to all spin-excitations. For the AKLT case, I even estimated this gap, using a single-mode approximation. Besides their intrinsic interest, these special systems highlighted the existence of two important classes of quantum manybody states - the Resonating Valence-Bond (RVB) state and the Valence-Bond Solid (VBS) state . As demonstrated in this chapter, these last states can be built for any lattice spin-system, by an appropriate Schwinger boson representation;
- In the **fifth and last chapter**, I have used the inspiration coming from the AKLT construction, to briefly introduce the more modern formalism of Tensor Product States, which is quickly being seen as a valuable resource in building efficient algorithms for studying strongly interacting manybody systems. In retrospect, this last chapter is the only one that truly deals with a

current line of research in this area, accomplishing a smooth connection between the established knowledge and future prospects for the author.

João Pedro dos Santos Pires

[This page was intentionally left blank]

Contents

1. The Heisenberg Model and Spin-Wave Theory **17**

1.1. The Heisenberg Model . . . 17
1.2. The Ferromagnetic Lattice and Spin-Wave Theory . . . 18
1.2.1. Low-Energy Spectrum and FM Spin-Waves . . . 20
1.2.2. Magnetization at Finite Temperatures . . . 22
1.3. The Heisenberg Antiferromagnet . . . 24
1.3.1. The Neél State and Quantum Effects . . . 24
1.3.2. AFM Spin-Wave Theory . . . 26
1.3.3. Destruction of Neél Order By Quantum Fluctuations . . . 29
1.3.4. Effect of Thermal Fluctuations . . . 30
1.4. Spin-Waves in the Graphene Lattice . . . 31
1.4.1. The Ferromagnetic Model . . . 31
1.4.1.1. Building the Spin-Wave Hamiltonian . . . 31
1.4.1.2. Diagonalizing the Spin-Wave Hamiltonian . . . 33
1.4.1.3. The Spin-Wave Dispersion Relation . . . 34
1.4.1.4. Spin-Spin Correlation Function and Interpretation of the Spin-Wave Branches . . . 35
1.4.1.5. Finite Temperature Properties . . . 37
1.4.2. The Antiferromagnetic Model . . . 38
1.4.2.1. Building the Spin-Wave Hamiltonian . . . 38
1.4.2.2. Diagonalizing the Hamiltonian . . . 39
1.4.2.3. Corrections to the Ground-State Energy and the Spin-Wave Dispersion Relation . . . 41
1.4.2.4. Correlation Functions and Interpretation of the Spin-Wave Modes . . . 42
1.4.2.5. Ground-State and Finite Temperature Magnetization . . . 44
1.4.3. Interpretation of the Spin-Wave Branches (Equation of Motion Method) . . . 45
1.4.4. The Easy-Axis Anisotropic AFM in the Graphene Lattice . . . 46
1.4.4.1. Building the Hamiltonian . . . 46
1.4.4.2. Diagonalizing the Hamiltonian . . . 47
1.5. The Failure of Spin-Wave Theory at Low-Dimensions (A Reflection) . . . 49

2. Magnetic Order and Exact Results in the Heisenberg Model **51**

2.1. What Is A Magnetically Ordered Phase? . . . 51
2.2. The Mermin-Wagner Theorem . . . 53
2.2.1. The Mermin-Wagner Bound in the Heisenberg Model . . . 54
2.2.2. Absence of order at $D = 1$ and $D = 2$ . . . 58

2.2.3. The Mermin-Wagner Theorem . . . 60
2.3. Some Exact Statements About The AFM Ground State . . . 61
2.3.1. Marshall's Theorem and Uniqueness of the Ground-State . . . 61
2.3.2. The Lieb-Schultz-Mattis Theorem for 1-D AFM Heisenberg Chain . . . 66
2.3.3. Generalization of the LSM Theorem to Higher-Dimensional Cubic Lattices . . . 69
2.4. Preliminary Conclusions and Open Questions . . . 71

3. Path-Integral Formulation of the Heisenberg Model 73
3.1. Quasi-Classical Spin States (Definition and Properties) . . . 73
3.1.1. Schwinger Bosons Representation . . . 73
3.1.2. Spin Coherent-States for a Single Spin . . . 74
3.1.3. Spin Coherent-States for a System of Many Spins . . . 78
3.2. Path-Integral Formulation for Lattice Spin Hamiltonians . . . 80
3.2.1. The Generating Functional Method . . . 80
3.2.2. Building the Spin Path-Integral . . . 81
3.3. The Haldane Mapping to the $\mathcal{O}(3)$ Non-Linear Sigma Model . . . 85
3.3.1. Continuum Approximation for the Spin Hamiltonian . . . 86
3.3.2. Continuum Approximation of the Geometrical Berry Phase . . . 89
3.3.3. Emergence of the Non-Linear Sigma Model . . . 90
3.4. One-Dimensional Models: The Θ-Term Topological Action . . . 92
3.5. The Haldane Conjecture . . . 93
3.5.1. Polyakov Renormalization Group (a Short Review) . . . 94
3.5.2. The Haldane Spectral Gap . . . 95

4. Exactly Solvable Quantum Spin Models 99
4.1. The Majumdar-Ghosh Model . . . 99
4.1.1. Building the Exact Ground-State . . . 99
4.1.2. Order and Correlations in the Ground-State . . . 102
4.1.2.1. Diagrammatic Approach: . . . 103
4.1.2.2. Correlation Function and 'Spin-Peierls' Order . . . 104
4.1.3. Are the Dimerized States the only Ground-States? . . . 105
4.1.4. The Thermodynamic Limit of the Majumdar-Ghosh Model . . . 107
4.1.5. The Low-Energy Spectrum of the Model . . . 108
4.1.5.1. The Fundamental Inequality . . . 113
4.2. The One-Dimensional AKLT Model . . . 117
4.2.1. Building the Ground-State . . . 118
4.2.2. The AKLT States in the Product Basis . . . 120
4.2.3. Order and Correlations in the AKLT Ground-States . . . 121
4.2.4. The Thermodynamic Limit of the AKLT Model . . . 123
4.2.5. The Low-Energy Spectrum of the AKLT Model . . . 127
4.2.6. The Schwinger Boson representation of the AKLT state . . . 132
4.2.7. Calculations of Correlation functions using a Spin Coherent-State Representation 134

4.2.8. What About the Excited States? . . . 138
4.2.8.1. The Single-Mode Approximation . . . 138
4.2.8.2. The SMA Dispersion Relation for the AKLT Model . . . 139
4.3. Generalizations of the VBS State . . . 140
4.3.1. The AKLT Construction In An Arbitrary Lattice . . . 140
4.3.2. The Parent Hamiltonian of a VBS state . . . 142
4.3.3. VBS Heuristics . . . 143
4.4. Summary . . . 144

5. Tensor Product States and Conclusions **145**
5.1. The Abstract MPS Construction . . . 145
5.1.1. Motivation . . . 145
5.1.2. The MPS Construction . . . 145
5.1.3. The Matrix Product States as an Efficient Variational Class . . . 148
5.1.4. The AKLT and MG Models as Examples of MPS . . . 149
5.2. Conclusions . . . 151

A. Appendix **153**
A.1. Lattice Sums and Discrete Fourier Transforms . . . 153
A.2. Proof of the Rotation Invariance of H_{Heis} . . . 154
A.3. Proof of the Holstein-Primakoff Representation . . . 155
A.4. Rotation of Spin Operators . . . 155
A.5. Diagonalization of the AFM Holstein-Primakoff Hamiltonian . . . 157

B. Appendix **159**
B.1. The Bogoliubov Inequality . . . 159
B.2. Exact Solution of the Infinite Range AFM Model . . . 160
B.3. Derivation of the Twisted Heisenberg Hamiltonian . . . 161

C. Appendix **163**
C.1. Properties of the Schwinger Bosons . . . 163
C.2. Heisenberg Uncertainty Relation Among Spin Components . . . 165
C.3. Orthogonality and Completeness Relations of the Spin Coherent States . . . 166
C.4. Representations in the Spin Coherent State Basis and Kutzner's Theorem . . . 169
C.4.1. Complex Plane Representation of Spin Coherent States . . . 169
C.4.2. Proof of Kutzner's Theorem on the Representation of Operators in the Coherent-State Basis . . . 170
C.4.3. Representation of the Spin Components in the Basis of Coherent States . . . 176
C.4.4. General Proof for the Expectation Values of Spin Operators in the Coherent-State Basis . . . 178
C.5. Derivation of the Correlation Functions from a Generating Functional . . . 179
C.6. Can the Partition Function be Written as a Trace over Spin Coherent-States? . . . 181
C.7. Auxiliary Calculations For The Haldane Mapping . . . 183

D. Appendix **187**
D.1. Calculation of the Overlaps between the AKLT States 187
D.2. Calculation of Spin Averages and Correlations in the AKLT States 188
D.3. Calculations for the proof of Lemma 6 191
D.4. SU(2) invariant combination of Schwinger Bosons 192
D.5. Calculation of the Double-Commutator for the SMA 193

1. The Heisenberg Model and Spin-Wave Theory

1.1. The Heisenberg Model

References: [7]

One of the most important spin models to be considered in the context of magnetism in solids, is the Heisenberg model. This model is generally given in a lattice $\mathscr{L}$ of spin, by the generic Hamiltonian (1.1).

$$H_{Heis} = \sum_{i,j\in\mathscr{L}} J(\overrightarrow{r}_j - \overrightarrow{r}_i)\overrightarrow{S}_i \cdot \overrightarrow{S}_j - \sum_{i\in\mathscr{L}} \overrightarrow{B}(\overrightarrow{r}_i) \cdot \overrightarrow{S}_i \tag{1.1}$$

Where $J(\overrightarrow{r}_j - \overrightarrow{r}_i)$ are the coupling parameters and $\overrightarrow{B}(\overrightarrow{r}_i)$ is a position dependent external magnetic field, which couples linearly with the spins. In the context of this work we will be mainly interested in the case where (1.1) only contains first-neighbor couplings and is invariant under lattice translations (i.e. $J(\overrightarrow{r}_j - \overrightarrow{r}_i) = J$). We will also drop the magnetic field term, reducing (1.1) to the simpler form (1.2):

$$H_{Heis} = J \sum_{<i,j>\in\mathscr{L}} \overrightarrow{S}_i \cdot \overrightarrow{S}_j \tag{1.2}$$

The symbols $\overrightarrow{S}_i = (S_i^x, S_i^y, S_i^z)$ in (1.2) stand for the usual quantum spin operators that respect the following non-commutative Lie algebra:

$$\left[S_i^a, S_j^b\right] = i\delta_{ij}\epsilon^{abc}S_i^c \tag{1.3}$$

The above algebra has an infinite number of irreducible representations which can be labeled by the eigenvalue $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...$ of the Casimir operator — $S_i^2 \equiv S_i^x S_i^x + S_i^y S_i^y + S_i^z S_i^z$. The standard basis for an $s-$representation (i.e an $2s+1$-dimensional one) of (1.3) is written as — $|s, m_s\rangle_i$ — and obeys the following:

$$S_i^2 \,|s, m_s\rangle_i = s(s+1)\,|s, m_s\rangle_i \tag{1.4}$$

$$S_i^z \,|s, m_s\rangle_i = m_s \,|s, m_s\rangle_i \tag{1.5}$$

For moving around in each representation, one can build the on-site ladder operators $S_i^{\pm} \equiv S_i^x \pm iS_i^y$ (note that $(S_i^+)^\dagger = S_i^-$), which have the following properties:

$$\left[S_i^{\pm}, S_i^z\right] = \mp S_i^{\pm}, \quad \left[S_i^+, S_i^-\right] = 2S_i^z, \quad \left[S_i^{\pm}, S_i^2\right] = 0, \quad \left[S_i^z, S_i^2\right] = 0 \tag{1.6}$$

$$S_i^{\pm} \left|s, m_s\right\rangle_i = \sqrt{s(s+1) - m_s(m_s \pm 1)} \left|s, m_s \pm 1\right\rangle_i \tag{1.7}$$

To better understand the structure of the Heisenberg Hamiltonian, it is useful to write it in terms of the basis of operators $\{S_i^+, S_i^-, S_i^z\}$, giving the following form:

$$H_{Heis} = J \sum_{<i,j>\in\mathscr{L}} \left[\frac{1}{2}\left\{S_i^+ S_j^- + S_i^- S_j^+\right\} + S_i^z S_j^z\right] \tag{1.8}$$

Before exploring possible solutions to the model (1.8), some considerations about symmetries are in order. It is trivial to see that the Heisenberg Hamiltonian is invariant under SU(2)-rotations, generated by the total spin operators $S_T^k \equiv \sum_{i\in\mathscr{L}} S_i^k$. A rotation of an angle α about an axis defined by the unit vector — $\hat{u} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ — is implemented by the action of the following unitary operator (1.9):

$$U(\alpha, \hat{u}) = \exp\{i\alpha\hat{u} \cdot \overrightarrow{S}_T\} \tag{1.9}$$

The commutator of (1.9) with H_{Heis} can be explicitly proven to be zero [Appendix A.2], in the case where $\overrightarrow{B} = 0$. This means that the model in question remains invariant under the simultaneous rotation of all the spins, which coincides with one's intuition that the energy only depends on its relative orientations. This means that the eigenstates of (1.8) can be chosen to be common eigenstates of both S_T^2 and S_T^z, i.e.:

$$|\Psi\rangle = |S, M_s, \alpha\rangle, \quad \text{with } 0 \leq S \leq Ns \tag{1.10}$$

N being the number of spins in the lattice and α representing the remaining quantum numbers needed to specify the state.

1.2. The Ferromagnetic Lattice and Spin-Wave Theory

References: [1,7,8]

If we consider the case where the Hamiltonian (1.8) has a negative coupling parameter ($J < 0$), the model is said to be **Ferromagnetic (FM)**. In the corresponding classical vector-model, we already know that the ground-state is any configuration where all the 'classical spins' are oriented in the same direction in space, spontaneously breaking the SU(2)-symmetry. But since our model is quantum, our

intuition begs verification. We can still make the educated guess that a ground-state wavefunction for the Heisenberg ferromagnet should be:

$$|GS\rangle_{\hat{z}} = \underset{i\in\mathscr{L}}{\otimes} |s,s\rangle_i = ... |s,s\rangle_{i-1} \otimes |s,s\rangle_i \otimes |s,s\rangle_{i+1} ... \in \mathscr{H}_s^{\otimes N} = \mathscr{H} \tag{1.11}$$

The state (1.11) is a simple product state, corresponding to a fully magnetized lattice in the $\hat{z}$-direction. Obviously, the direction of magnetization is immaterial, since the Heisenberg ferromagnet has an SU(2)-symmetry. Hence, if $|GS\rangle_{\hat{z}}$ is a ground-state of the system, so will be any other state obtained by applying an arbitrary rotation operator to it. Using the definition (1.9), we can obtain all those states as:

$$|GS\rangle_{\alpha,\hat{u}} = U(\alpha,\hat{u}) \left[... |s,s\rangle_{i-1} \otimes |s,s\rangle_i \otimes |s,s\rangle_{i+1} ...\right] = \otimes_{i\in\mathscr{L}} \left[e^{i\alpha\hat{u}\cdot\overrightarrow{S}_i} |s,s\rangle_i\right] \tag{1.12}$$

They are all unentangled states. Now, to prove that (1.11) is indeed a ground-state of the model, we start by checking that (1.11) is an eigenstate of (1.8):

$$H_{Heis} |GS\rangle_{\hat{z}} = J \sum_{<i,j>\in\mathscr{L}} \left[\frac{1}{2}\left\{S_i^+ S_j^- + S_i^- S_j^+\right\} + S_i^z S_j^z\right] |GS\rangle_{\hat{z}} = J \sum_{<i,j>\in\mathscr{L}} s^2 |GS\rangle_0 = -|J| z N s^2 |GS\rangle_{\hat{z}} \tag{1.13}$$

Where z is the coordination of the lattice and N is the number of spins. To obtain (1.13), we made use of the fact that any raising operator acting on $|GS\rangle_{\hat{z}}$ will give annihilate it, meaning that the only contribution comes from $S_i^z S_j^z |GS\rangle_{\hat{z}} = s^2 |GS\rangle_{\hat{z}}$.

At last, we need to prove that — $E_0 = -|J| z N s^2$ — is really the minimum eigenvalue of the Hamiltonian. To do it, we just use the following rigorous bound[1]:

$$-s(s+1) \leq \langle\Psi| \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j |\Psi\rangle \leq s^2 \tag{1.14}$$

Where $|\Psi\rangle$ is any state of $\mathscr{H}$. Applying this inequality to $\langle\Psi| H_{Heis} |\Psi\rangle$, one gets:

$$-zNs(s+1) \leq \langle\Psi| \sum_{\langle i,j\rangle\in\mathscr{L}} \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j |\Psi\rangle \leq zNs^2$$

Meaning that — $\langle\Psi| H_{Heis} |\Psi\rangle \geqslant -|J| z N s^2$ and therefore $|GS\rangle_{\hat{z}}$ must be a ground-state of H_{Heis}. By symmetry, the ground-state manifold is infinitely-dimensional and composed of states that break the rotational symmetry.

[1] To prove this bound is enough to write:

$$\left(\overrightarrow{\mathbf{S}}_i + \overrightarrow{\mathbf{S}}_j\right)^2 = S_i^2 + S_j^2 + 2\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j$$

Taking the average in any state (with total spin s) and knowing that any state in $\mathscr{H}_i \otimes \mathscr{H}_j$ has total spin between 0 and $2s$, one gets the desired result (1.14).

1.2.1. Low-Energy Spectrum and FM Spin-Waves

Knowing the exact ground-state of the Heisenberg FM is a very important piece of information, but is not enough to make any physical predictions at finite temperatures. For that, one must also know the low-energy spectrum and the corresponding excited states. That need leads us to introduce the formalism of **Spin-Wave Theory**, developed in the 1940's, mainly by T. Holstein and H. Primakoff [1].

To start, we notice that the Hamiltonian (1.8) is not attached to any particular representation of the spin operators. Therefore, one is allowed to write the operators $\{S_i^+, S_i^-, S_i^z\}$ in any way, as long as the commutation relations between them are preserved. In [Appendix A.3], it is proven that the bosonic representation (1.15) is a legitimate way of writing the spin operators. The operators $a_i/a_i^\dagger$ are known as the **Holstein-Primakoff operators**.

$$S_i^z = s - a_i^\dagger a_i, \quad S_i^+ = \sqrt{2s - a_i^\dagger a_i}\, a_i, \quad S_i^- = a_i^\dagger \sqrt{2s - a_i^\dagger a_i} \tag{1.15}$$

$$\left[a_i, a_j^\dagger\right] = \delta_{ij}\mathbb{I}, \quad \left[a_i^\dagger a_i, a_i\right] = -a_i, \quad \left[a_i^\dagger a_i, a_i^\dagger\right] = a_i^\dagger$$

We could plug in the expressions (1.15) into the Heisenberg Hamiltonian and arrive at a perfectly good representation for a spin-s model. However, the square-roots in the ladder operators would greatly complicate the expression of H_{Heis} and, to make actual calculations, people usually expand the square-roots in (1.15) as powers of $1/s$, i.e.:

$$\sqrt{2s - a_i^\dagger a_i} \approx \sqrt{2s}\left\{1 - \frac{a_i^\dagger a_i}{4s} + ...\right\} \Longrightarrow \begin{cases} S_i^+ = \sqrt{2s}\left\{a_i - \frac{a_i^\dagger a_i a_i}{4s} + ...\right\} \\ S_i^- = \sqrt{2s}\left\{a_i^\dagger - \frac{a_i^\dagger a_i^\dagger a_i}{4s} + ...\right\} \end{cases} \tag{1.16}$$

This procedure is approximate and explicitly disrespects the required spin algebra. In particular, it allows the ladder operators to create an arbitrarily large number of local spin excitations, thus violating the constraint that $s \geq m_s \geq -s$. This would not be a problem in the large-s limit[2] but, for the (usual) situation where s is of the order of unity, it is hardly justifiable. Anyway, its success in describing most of the experimental phenomena fully justifies the usefulness of this simplification for our following discussion.

Using (1.16), the Heisenberg Hamiltonian takes the form:

[2] This limit corresponds to the case where the spins in the lattice sites are classical spins. That can be easily seen by the following argument:

- If we normalize the spin operators as — $\widetilde{S}_i^k = \frac{1}{s} S_i^k$ — then the average value of $\widetilde{S}_i^k$ in any state will always lie between -1 and 1;
- Then, we can write the commutator between the spin components as — $\left[\widetilde{S}_i^{k_1}, \widetilde{S}_i^{k_2}\right] = \frac{i}{s}\epsilon^{k_1 k_2 k_3}\widetilde{S}_i^{k_3} \xrightarrow[s\to\infty]{} 0$

This last limit indicates that the uncertainty relation between the spin components becomes irrelevant for large s and the spins behave as classical 3-vectors. This statement can be made even more precise by working directly with the partition function — Z_s — associated with the quantum spin model. This was done by E. Lieb in [18], using a spin coherent-state formalism that allowed the derivation of precise bounds on Z_s and prove that $\lim_{s\to\infty} Z_s = Z_{cl}$.

$$H_{Heis} = J \sum_{<i,j>} \Bigg\{ s \left[a_i - \frac{a_i^\dagger a_i a_i}{4s} + ... \right] \left[a_j^\dagger - \frac{a_j^\dagger a_j^\dagger a_j}{4s} + ... \right] + s \left[a_i^\dagger - \frac{a_i^\dagger a_i^\dagger a_i}{4s} + ... \right] \times$$
$$\times \left[a_j - \frac{a_j^\dagger a_j a_j}{4s} + ... \right] + \left[s - a_i^\dagger a_i \right] \left[s - a_j^\dagger a_j \right] \Bigg\} = Js^2 \sum_{<i,j>} \Bigg\{ 1 + \frac{1}{s} \Bigg[a_i a_j^\dagger - \frac{a_i^\dagger a_i a_i a_j^\dagger}{4s} -$$
$$- \frac{a_i a_j^\dagger a_j^\dagger a_j}{4s} + a_i^\dagger a_j - \frac{a_i^\dagger a_i^\dagger a_i a_j}{4s} - \frac{a_i^\dagger a_j^\dagger a_j a_j}{4s} - a_i^\dagger a_i - a_j^\dagger a_j \Bigg] + \mathcal{O}(\frac{1}{s^3}) \Bigg\}$$

Separating the non-interacting part from the rest, we get:

$$H_{Heis} = E_0 + Js \sum_{<i,j>} \Big\{ a_i a_j^\dagger + a_i^\dagger a_j - a_i^\dagger a_i - a_j^\dagger a_j \Big\} + H_{Int} \tag{1.17}$$

This new effective Hamiltonian describes the dynamics of the low-lying spin excitations above the FM ground-state. If one ignores the interaction terms (which can be treated in perturbation theory), (1.17) reduces to a quadratic Hamiltonian, which can be diagonalized in momentum-space. For the calculations, we will resort to the definitions given in the [Appendix A.1], but using the following normalizations that ensure bosonic commutation relations for the $a_{\mathbf{k}}$ operators:

$$\begin{cases} a_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in FBZ} a_{\mathbf{k}} e^{-i \mathbf{R_j} \cdot \mathbf{k}} \\ a_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in FBZ} a_{\mathbf{k}}^\dagger e^{i \mathbf{R_j} \cdot \mathbf{k}} \end{cases} \Longrightarrow \begin{cases} a_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j \in \mathscr{L}} a_j e^{i \mathbf{R_j} \cdot \mathbf{k}} \\ a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j \in \mathscr{L}} a_j^\dagger e^{-i \mathbf{R_j} \cdot \mathbf{k}} \end{cases} \tag{1.18}$$

To apply this change of basis to the effective Hamiltonian (1.17), we parametrize the sum over first-neighbors as follows:

$$H_{SW} = -\left|J\right| s \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}} \sum_{\alpha=1}^{z} \Big\{ a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i - \vec{\delta}_\alpha) + a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i + \vec{\delta}_\alpha) - 2 a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i) \Big\} \tag{1.19}$$

And notice also that:

$$\sum_{\vec{\mathbf{R}} \in \mathscr{L}} \sum_{\vec{\mathbf{G}}} a^\dagger(\vec{\mathbf{R}}) a(\vec{\mathbf{R}} + \vec{\delta}) = \frac{1}{N} \sum_{\vec{\mathbf{R}} \in \mathscr{L}} \sum_{\vec{\delta}} \sum_{\vec{\mathbf{q}} \in FBZ} \sum_{\vec{\mathbf{k}} \in FBZ} a_{\vec{\mathbf{q}}}^\dagger a_{\vec{\mathbf{k}}} e^{i \vec{\mathbf{R}} \cdot (\vec{\mathbf{q}} - \vec{\mathbf{k}})} e^{-i \vec{\delta} \cdot \vec{\mathbf{k}}}$$
$$= \frac{(2\pi)^d}{N v_{cell}} \sum_{\vec{\delta}} \sum_{\vec{\mathbf{q}} \in FBZ} \sum_{\vec{\mathbf{k}} \in FBZ} a_{\vec{\mathbf{q}}}^\dagger a_{\vec{\mathbf{k}}} e^{-i \vec{\delta} \cdot \vec{\mathbf{k}}} \sum_{\vec{\mathbf{K}} \in \mathscr{L}^*} \delta^{(d)}(\vec{\mathbf{q}} - \vec{\mathbf{k}} - \vec{\mathbf{K}})$$
$$= \frac{(2\pi)^d}{N v_{cell}} \sum_{\vec{\mathbf{q}} \in FBZ} \sum_{\vec{\mathbf{k}} \in FBZ} \gamma_{\vec{\mathbf{k}}} a_{\vec{\mathbf{q}}}^\dagger a_{\vec{\mathbf{k}}} \delta^{(d)}(\vec{\mathbf{q}} - \vec{\mathbf{k}}) = \sum_{\vec{\mathbf{k}} \in FBZ} \gamma_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}}^\dagger a_{\vec{\mathbf{k}}} \tag{1.20}$$

Where — $\gamma_{\vec{\mathbf{k}}} = \sum_{\vec{\delta}} e^{-i \vec{\delta} \cdot \vec{\mathbf{k}}}$ — and use was made of the first lattice sum — (A.3) — in [Appendix A.1]. Using (1.20) in each of the terms of (1.19) yields:

$$H_{SW} = -\left|J\right| s \sum_{\vec{\mathbf{k}} \in FBZ} a^{\dagger}_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} \left\{ \gamma_{-\vec{\mathbf{k}}} + \gamma_{\vec{\mathbf{k}}} - 2z \right\} \tag{1.21}$$

We see that (1.21) is a diagonal Hamiltonian and by calling $\vec{\delta}_{\alpha}$ the first-neighbor vectors, we get the following gapless dispersion relation:

$$\epsilon(\vec{\mathbf{k}}) = -2\left|J\right| s \left[\sum_{\alpha=1}^{z} \cos\left(\delta_{\alpha} \cdot \vec{\mathbf{k}} \right) - z \right] \approx \left|J\right| s \sum_{\alpha=1}^{z} \left(\delta_{\alpha} \cdot \vec{\mathbf{k}} \right)^2 + ... \tag{1.22}$$

As an example, we have calculated the dispersion relation for the cases of the 1-D chain and also the 2-D rectangular lattice. The results are:

$$\epsilon_{1D}(k) = -4\left|J\right| s \left[\cos\left(ak\right) - 1\right] \approx 2a^2 \left|J\right| sk^2 + ... \tag{1.23}$$

$$\epsilon_{Rect}(k_x, k_y) = -4\left|J\right| s \left[\cos\left(ak_x\right) + \cos\left(bk_y\right) - 2\right] \approx 2\left|J\right| s(a^2 k_x^2 + b^2 k_y^2) + ... \tag{1.24}$$

Notice that in all the cases above, the low-energy excitations are also low-momentum states (i.e. states with $\vec{\mathbf{k}}$ near the Γ-point).

1.2.2. Magnetization at Finite Temperatures

With the knowledge of the low-energy spectrum for the model Hamiltonian, we can calculate thermodynamic quantities at finite (but low) temperatures. In what follows, we will assume that we are working in an hyper-cubic lattice in d-dimensions, such that the dispersion relation for the hydrodynamic spin-waves takes the isotropic form:

$$\epsilon(k) = E_0 + 2\left|J\right| sa^2 \left|\vec{\mathbf{k}}\right|^2, \quad for \ \left|\vec{\mathbf{k}}\right| \ll \frac{1}{a} \tag{1.25}$$

In the free-magnon approximation, the quantum state of the system, at temperature T, is given in the form of the canonical density operator (1.26).[3]

$$\rho(\beta) = \frac{1}{Z(\beta)} \exp\left[-\beta \sum_{\vec{\mathbf{k}} \in FBZ} (\epsilon(k) - E_0) a^{\dagger}_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} \right] = \frac{\exp\left[-\beta \sum_{\vec{\mathbf{k}} \in FBZ} (\epsilon(k) - E_0) a^{\dagger}_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} \right]}{Tr\left[\exp\left[-\beta \sum_{\vec{\mathbf{k}} \in FBZ} (\epsilon(k) - E_0) a^{\dagger}_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} \right] \right]} \tag{1.26}$$

Right away, we can use (1.26) to calculate the average uniform magnetization on the lattice. The magnetization is the volume density of magnetic-moment, which means that:

[3] The apparent paradox in using the approximate dispersion relation (1.25) is rendered irrelevant by the exponential suppression of the big-k Spin-Waves.

$$
\begin{aligned}
M^z &= \frac{1}{Nv_{cell}}\left\langle \sum_{i\in\mathscr{L}} S_i^z \right\rangle_T = \frac{1}{Nv_{cell}} Tr\left[\rho(\beta)\sum_{\vec{\mathbf{R}}\in\mathscr{L}}\left\{s - a^\dagger(\vec{\mathbf{R}})a(\vec{\mathbf{R}})\right\}\right] \\
&= \frac{s}{v_{cell}} - \frac{1}{Nv_{cell}} Tr\left[\rho(\beta)\sum_{\vec{\mathbf{R}}\in\mathscr{L}}\left\{a^\dagger(\vec{\mathbf{R}})a(\vec{\mathbf{R}})\right\}\right] = \\
&= \frac{s}{v_{cell}} - \frac{1}{Nv_{cell}}\sum_{\vec{\mathbf{k}}\in FBZ} Tr\left[\rho(\beta)a^\dagger_{\vec{\mathbf{k}}}a_{\vec{\mathbf{k}}}\right] = \frac{s}{v_{cell}} - \frac{1}{Nv_{cell}}\sum_{\vec{\mathbf{k}}\in FBZ}\left\langle n_{\vec{\mathbf{k}}}\right\rangle
\end{aligned} \tag{1.27}
$$

Since the spin-waves are bosonic excitations, the average value of the occupation numbers, in equilibrium, is given by the Planck Distribution:

$$
\begin{aligned}
M^z &= \frac{s}{v_{cell}} - \frac{1}{Nv_{cell}}\sum_{\mathbf{k}\in FBZ}\frac{1}{\exp\left[2\beta\left|J\right|sa^2k^2\right]-1} \rightarrow \\
&\rightarrow \frac{s}{v_{cell}} - \frac{1}{(2\pi)^d}\int_{FBZ} d^d\mathbf{k}\frac{1}{\exp\left[2\beta s\left|J\right|a^2k^2\right]-1} =
\end{aligned} \tag{1.28}
$$

To make a numerical estimate of this thermal correction, we can extend the momentum integral to all of the $\vec{\mathbf{k}}$-space and also introduce an 'infrared' momentum cut-off λ (that will allow us to parametrize eventual divergences in the large-wavelength region). Since the integrand is isotropic, the angular integration is trivial and one gets:

$$
M^z = M_0^z - \Delta M^z = \frac{s}{v_{cell}} - \frac{S_{d-1}}{(2\pi)^d}\int_\lambda^{+\infty} dk\frac{k^{d-1}}{\exp\left[2\beta s\left|J\right|a^2k^2\right]-1} \tag{1.29}
$$

Where S_{d-1} is the surface area of the $(n-1)$-dimensional unit sphere[4]. The integral in (1.29) is always convergent for large k, but for small k the situation depends crucially on the dimensionality of the lattice. To see that, we can derive a low-k asymptotic expression for the integrand, as follows:

$$
\Delta M^z = \frac{S_{d-1}}{(2\pi)^d}\int_\lambda^{+\infty} dk\frac{k^{d-1}}{\exp\left[2\beta\left|J\right|sa^2k^2\right]-1} \approx \frac{1}{2\beta\left|J\right|sa^2}\int_\lambda^{+\infty} dkk^{d-3} \tag{1.30}
$$

From (1.30), it can be seen that for $d = 1, 2$, the correction to the ground-state magnetization, due to the spin-waves is divergent. This situation indicates the absence of ferromagnetic order in 1- and 2-dimensional Heisenberg Models at $T \neq 0K$, which is a general result for spin systems with short-ranged interactions (this is called Mermin-Wagner's Theorem and will be discussed in Chapter 2). In the 3-dimensional cubic lattice, we get the following result:

$$
M^z = M_0^z - \Delta M^z = \frac{s}{v_{cell}} - \frac{1}{2\pi^2}\int_0^{+\infty} dk\frac{k^2}{\exp\left[2\beta\left|J\right|sa^2k^2\right]-1} = \frac{s}{a^3} - \zeta(3/2)\frac{\sqrt{\pi}}{8\pi(2\left|J\right|s\beta a^2)^{3/2}} \tag{1.31}
$$

[4]This value is known to be $S_{d-1} = \frac{(2\pi)^{d/2}}{\Gamma(d/2)}$.

This last expression can be recasted in the form of the famous Bloch's Law for the dependence of the magnetization with temperature:

$$M^z(T) = M_0^z \left(1 - \left(\frac{T}{T_C}\right)^{\frac{3}{2}}\right) \tag{1.32}$$

With:

$$T_C = \frac{8s}{\zeta(3/2)} \left(\frac{2\pi |J| s}{k_B}\right)^{3/2}$$

.

1.3. The Heisenberg Antiferromagnet

References: [2,3,6,7,8]

1.3.1. The Neél State and Quantum Effects

Now, we turn our attention to the **Antiferromagnetic** case (AFM) (where $J > 0$), and we will try to follow the same path as in the last section. For simplicity, we will consider the Heisenberg Hamiltonian (1.2) in a d-dimensional hypercubic lattice, which is a **bipartite lattice**.[5]

For a start, we need to determine the ground-state manifold for this system. Building on classical intuition, one can propose the **Neél State** as an 'ansatz' for the ground-state of H_{Heis}:

$$|\Psi_{Néel}\rangle = \bigotimes_{i \in \mathscr{L}} |s, \eta_i s\rangle_i \,, \quad \text{where } \eta_i = \begin{cases} 1 & i \in \mathscr{L}_A \\ -1 & i \in \mathscr{L}_B \end{cases} \tag{1.33}$$

Now, we can test to see if (1.33) is an eigenstate of the Hamiltonian. For that, we can rewrite the Hamiltonian as:

$$H_{Heis} = J \sum_{\langle i,j \rangle \in \mathscr{L}} \left[\frac{1}{2}\left\{S_i^+ S_j^- + S_i^- S_j^+\right\} + S_i^z S_j^z\right] = 2J \sum_{i \in \mathscr{L}_A} \sum_{j \in viz(i)} \left[\frac{1}{2}\left\{S_i^+ S_j^- + S_i^- S_j^+\right\} + S_i^z S_j^z\right] \tag{1.34}$$

Which means that:

[5] A bipartite lattice is a lattice that can be seen as two interpenetrating sublattices, i.e. $\mathscr{L} = \mathscr{L}_A \oplus \mathscr{L}_B$. This excludes the phenomenon of classical frustration (as happens in the 2-D triangular lattice, for example) which excludes the Néel State as a classical ground state.

$$
\begin{aligned}
H_{Heis}\left|\Psi_{N\acute{e}el}\right\rangle &= 2J\sum_{i\in\mathscr{L}_A}\sum_{j\in viz(i)}\left\{...\otimes\left[\left[\frac{1}{2}\left\{S_i^+S_j^- + S_i^-S_j^+\right\} + S_i^zS_j^z\right]\left|s,s\right\rangle_i\otimes\left|s,-s\right\rangle_i\right]\otimes...\right\} \\
&= J\sum_{i\in\mathscr{L}_A}\sum_{j\in viz(i)}\left\{...\otimes\left[S_i^-S_j^+\left|s,s\right\rangle_i\otimes\left|s,-s\right\rangle_i\right]\otimes...\right\} - JzNs^2\left|\Psi_{N\acute{e}el}\right\rangle \\
&= 2J\sum_{i\in\mathscr{L}_A}\sum_{j\in viz(i)}\left\{...\otimes\left|s,s-1\right\rangle_i\otimes\left|s,-s+1\right\rangle_i\otimes...\right\} - JzNs^2\left|\Psi_{N\acute{e}el}\right\rangle \qquad (1.35)
\end{aligned}
$$

Obviously, all the states in the sum of (1.35) are orthogonal among them and also orthogonal to $|\Psi_{N\acute{e}el}\rangle$. Hence, $|\Psi_{N\acute{e}el}\rangle$ cannot be an eigenstate of H_{Heis} . This means that, unlike the FM case, here the classical lowest-energy configuration does not correspond to the correct ground-state of the related quantum model.[6]

Our 'ansatz' failed this time, because the **Staggered Magnetization Operator** — $S_{Neél} = S_z^{(A)} - S_z^{(B)}$[7] — does not commute with the Hamiltonian (1.2). This can be proven by a direct calculation, as follows:

$$
\begin{aligned}
\left[S_z^{(A)}, H_{Heis}\right] &= J\sum_{\langle i,j\rangle\in\mathscr{L}}\left\{S_j^x\left[S_z^{(A)},S_i^x\right] + S_j^y\left[S_z^{(A)},S_i^y\right]\right\} = \\
&= J\sum_{\langle i,j\rangle\in\mathscr{L}}\sum_{k\in\mathscr{L}_A}\left\{S_j^x\left[S_k^z,S_i^x\right] + S_j^y\left[S_k^z,S_i^y\right]\right\} = \\
&= iJ\sum_{\langle i,j\rangle\in\mathscr{L}}\sum_{k\in\mathscr{L}_A}\delta_{ik}\left\{S_j^xS_i^y - S_j^yS_i^x\right\} = iJ\sum_{\langle i,j\rangle\in\mathscr{L}}\left\{S_j^xS_i^y - S_j^yS_i^x\right\}
\end{aligned}
$$

$$
\begin{aligned}
\left[S_z^{(B)}, H_{Heis}\right] &= J\sum_{\langle i,j\rangle\in\mathscr{L}}\left\{\left[S_z^{(B)},S_j^x\right]S_i^x + \left[S_z^{(B)},S_j^y\right]S_i^y\right\} = \\
&= J\sum_{\langle i,j\rangle\in\mathscr{L}}\sum_{k\in\mathscr{L}_B}\left\{S_i^x\left[S_k^z,S_j^x\right] + S_i^y\left[S_k^z,S_j^y\right]\right\} = \\
&= iJ\sum_{\langle i,j\rangle\in\mathscr{L}}\sum_{k\in\mathscr{L}_B}\delta_{jk}\left\{S_i^xS_j^y - S_i^yS_j^x\right\} = iJ\sum_{\langle i,j\rangle}\left\{S_i^xS_j^y - S_i^yS_j^x\right\}
\end{aligned}
$$

Which yields $[S_{Neél}, H_{Heis}] = 2iJ\sum_{\langle i,j\rangle}\left\{S_i^xS_j^y - S_i^yS_j^x\right\} \neq 0$. This non-commutativity implies that the quantum numbers associated with the eigenvectors of $S_{Neél}$ — the Neél States — are not good quantum numbers, for the Heisenberg model. Despite this complication, it turns out [2,3] that we may still assume that the ground-state exhibits some kind of (imperfect) staggered magnetization and therefore build a Spin-Wave Theory around the Néel state.

[6] Notice that in the limit $s \to \infty$ of equation (1.35), the Néel state is, indeed, the correct ground state, reproducing the expected classical result.

[7] Where (A) and (B) refer to the two sublattices.

1.3.2. AFM Spin-Wave Theory

The Neél state is very different from the ferromagnetic state, but still we can turn one into the other by applying a π *rad* rotation around the y-axis, for the spins in the sublattice B. The effect of this rotation in the spin operators is [Appendix A.4]:

$$\widetilde{S}_i^z = e^{i\pi S_i^y} S_i^z e^{-i\pi S_i^y} = -S_i^z; \quad \widetilde{S}_i^{\pm} = e^{i\pi S_i^y} S_i^{\pm} e^{-i\pi S_i^y} = -S_i^{\mp} \tag{1.36}$$

Trivially, the operators in (1.36) still obey the correct algebra:

$$\left[\widetilde{S}_i^{\pm}, \widetilde{S}_i^z\right] = \mp \widetilde{S}_i^{\pm}, \quad \left[\widetilde{S}_i^{+}, \widetilde{S}_i^{-}\right] = 2\widetilde{S}_i^z \quad and \quad \widetilde{S}_i^z \left|\Psi_{N\acute{e}el}\right\rangle = s \left|\Psi_{N\acute{e}el}\right\rangle \tag{1.37}$$

Therefore, one can represent the operators (1.36) in terms of Holstein-Primakoff operators, just as in the last section. In this case, the correct correspondence (such that $|\Psi_{N\acute{e}el}\rangle$ is the basis for the expansion[8]) is the following:

$$\begin{aligned} &S_i^z = s - a_i^\dagger a_i, \quad S_i^+ = \sqrt{2s - a_i^\dagger a_i}\, a_i, \quad S_i^- = a_i^\dagger \sqrt{2s - a_i^\dagger a_i}; \quad if\, i \in \mathscr{L}_A \\ &S_i^z = -s + b_i^\dagger b_i, \quad S_i^- = -\sqrt{2s - b_i^\dagger b_i}\, b_i, \quad S_i^+ = -b_i^\dagger \sqrt{2s - b_i^\dagger b_i}; \quad if\, i \in \mathscr{L}_B \end{aligned} \tag{1.38}$$

Once again, we make a $1/s$ expansion to first order, yielding:

$$\begin{aligned} &S_i^z = s - a_i^\dagger a_i, \quad S_i^+ \approx \sqrt{2s}\, a_i, \quad S_i^- \approx \sqrt{2s}\, a_i^\dagger; \quad if\, i \in \mathscr{L}_A \\ &S_i^z = -s + b_i^\dagger b_i, \quad S_i^- \approx -\sqrt{2s}\, b_i, \quad S_i^+ \simeq -\sqrt{2s}\, b_i^\dagger \quad if\, i \in \mathscr{L}_B \end{aligned} \tag{1.39}$$

We then apply (1.39) to the Hamiltonian (1.34), ending up with:

$$\begin{aligned} H_{Heis} &= 2J \sum_{i \in \mathscr{L}_A} \sum_{j \in viz(i)} \left[\frac{1}{2}\left\{S_i^+ S_j^- + S_i^- S_j^+\right\} + S_i^z S_j^z\right] = \\ &= -2J \sum_{i \in \mathscr{L}_A} \sum_{j \in viz(i)} \left[s\left\{a_i b_j + a_i^\dagger b_j^\dagger\right\} + (s - a_i^\dagger a_i)(s - b_j^\dagger b_j)\right] + ... = \\ &= -Js^2 Nz - 2Js \sum_{i \in \mathscr{L}_A} \sum_{j \in viz(i)} \left[a_i b_j + a_i^\dagger b_j^\dagger - a_i^\dagger a_i - b_j^\dagger b_j\right] + ... = \\ &= -Js^2 Nz - 2Js \left\{\sum_{i \in \mathscr{L}_A} \sum_{j \in viz(i)} \left[a_i b_j + a_i^\dagger b_j^\dagger\right] - z \sum_{i \in \mathscr{L}_A} a_i^\dagger a_i - z \sum_{j \in \mathscr{L}_B} b_j^\dagger b_j\right\} + ... \end{aligned} \tag{1.40}$$

[8] Note that the representation given in (1.38) guarantees that $a_i^\dagger$ decreases a quantum of spin from the site $i \in \mathscr{L}_A$, while $b_i^\dagger$ increases the same amount in the site $i \in \mathscr{L}_B$. In both cases, the creation of a or b bosons, act to decrease the staggered magnetization, as expected.

A comparison between (1.40) and (1.17), unveils that the AFM effective Hamiltonian contains 'anomalous' terms — $a_i b_j$ and $a_i^\dagger b_j^\dagger$ — that do not conserve the number of bosons in the system. This is just an expression of the inadequacy of $|\Psi_{N\acute{e}el}\rangle$, as a legitimate ground-state for the model.

We now move to momentum-space, transforming term-by-term, as follows[9]:

$$\sum_{\vec{\mathbf{R}}\in\mathscr{L}_A} a^\dagger(\vec{\mathbf{R}})a(\vec{\mathbf{R}}) = \sum_{\vec{\mathbf{k}}\in FBZ_{sub}} a^\dagger_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}}; \quad \sum_{\vec{\mathbf{R}}\in\mathscr{L}_B} b^\dagger(\vec{\mathbf{R}})b(\vec{\mathbf{R}}) = \sum_{\vec{\mathbf{k}}\in FBZ_{sub}} b^\dagger_{\vec{\mathbf{k}}} b_{\vec{\mathbf{k}}} \tag{1.41}$$

$$\sum_{\vec{\mathbf{R}}\in\mathscr{L}_A}\sum_\alpha a^\dagger(\vec{\mathbf{R}})b^\dagger(\vec{\mathbf{R}}+\vec{\delta}_\alpha) = \sum_{\vec{\mathbf{k}}\in FBZ_{sub}} \gamma_{-\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}} b^\dagger_{-\vec{\mathbf{k}}}$$

$$\sum_{\vec{\mathbf{R}}\in\mathscr{L}}\sum_\alpha a(\vec{\mathbf{R}})b(\vec{\mathbf{R}}+\vec{\delta}_\alpha) = \sum_{\vec{\mathbf{k}}\in FBZ_{sub}} \gamma_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}} b^\dagger_{-\vec{\mathbf{k}}} \tag{1.42}$$

Where $\vec{\delta}_\alpha$ are the position vectors that connect the site $\vec{\mathbf{R}} \in \mathscr{L}_A$ to each one of its first-neighbors (all belonging to $\mathscr{L}_B$) and $\gamma_{\vec{\mathbf{k}}} = \sum_\alpha e^{-i\vec{\delta}_\alpha\cdot\vec{\mathbf{k}}} = \gamma_{-\vec{\mathbf{k}}}$ for the case of a lattice with inversion symmetry[10] around each node. Using (1.41) and (1.42) into the Hamiltonian (1.40), we finally get:

$$H_{SW} = H_{Heis} + Js^2Nz = -2Jzs \sum_{\vec{\mathbf{k}}\in FBZ_{sub}} \left\{ \frac{\gamma_{\vec{\mathbf{k}}}}{z}\left[a_{\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}} + a^\dagger_{\vec{\mathbf{k}}} b^\dagger_{-\vec{\mathbf{k}}}\right] - \left[b^\dagger_{\vec{\mathbf{k}}} b_{\vec{\mathbf{k}}} + a^\dagger_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}}\right]\right\} \tag{1.43}$$

Unfortunately, the non-conserving terms prevent (1.43) from being diagonal. Hence, to complete the diagonalization one must perform a **Bogoliubov-Valatin Tranformation**, similar to the one used to diagonalize the BCS effective Hamiltonian, in the theory of normal superconductivity. Proceeding with this, we can define the new bosonic operators as in (1.44) (with $u_{\vec{\mathbf{k}}} = u_{-\vec{\mathbf{k}}}$ and $v_{\vec{\mathbf{k}}} = v_{-\vec{\mathbf{k}}}$):

$$\begin{cases} c_{\vec{\mathbf{k}}} = u_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} - v_{\vec{\mathbf{k}}} b^\dagger_{-\vec{\mathbf{k}}} \\ c^\dagger_{\vec{\mathbf{k}}} = u^*_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}} - v^*_{\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}} \end{cases} \qquad \begin{cases} d_{\vec{\mathbf{k}}} = u_{\vec{\mathbf{k}}} b_{\vec{\mathbf{k}}} - v_{\vec{\mathbf{k}}} a^\dagger_{-\vec{\mathbf{k}}} \\ d^\dagger_{\vec{\mathbf{k}}} = u^*_{\vec{\mathbf{k}}} b^\dagger_{\vec{\mathbf{k}}} - v^*_{\vec{\mathbf{k}}} a_{-\vec{\mathbf{k}}} \end{cases} \tag{1.44}$$

The general transformation (1.44) is required to preserve the bosonic commutation relations among the involved operators (it is a Canonical Transformation), i.e. $\left[d_{\mathbf{k_1}}, d^\dagger_{\mathbf{k_2}}\right] = \delta_{k_1k_2}$, $\left[c_{\mathbf{k_1}}, c^\dagger_{\mathbf{k_2}}\right] = \delta_{k_1k_2}$ and $\left[c_{\mathbf{k_1}}, d^\dagger_{\mathbf{k_2}}\right] = \left[d_{\mathbf{k_1}}, c^\dagger_{\mathbf{k_2}}\right] = 0$. Imposing these conditions on the commutators, the only non-trivial constraint for the functions $u_{\tilde{\mathbf{k}}}$ and $v_{\vec{\mathbf{k}}}$ will be:

$$\left[c_{\vec{\mathbf{k}}}, c^\dagger_{\vec{\mathbf{k}}}\right] = 1 \Longrightarrow \left|u_{\vec{\mathbf{k}}}\right|^2 - \left|v_{\vec{\mathbf{k}}}\right|^2 = 1 \tag{1.45}$$

[9] We must also take notice that here the sums over $\mathbf{k}$ are performed over the First Brillouin Zone of a sublattice, whose sides are only half of the the size of the FBZ for the whole lattice. Therefore, if $\mathscr{L}$ has N unit cells with periodic boundary conditions, there will be two magnon branches, but each one will have only $N/2$ possible crystal momenta. Thus, in the end, the total number of different magnon states is still N.

[10] The rest of the calculations in this section are only valid in this case. However, in the practical exercise of Section 1.4, we have dealt with a case in which $\gamma_{\vec{\mathbf{k}}}$ is not a real number, to show that everything works the same way, only with some extra technical complications in parametrizing the BV Transformation.

Furthermore, we also require (1.44) to do the intended job of diagonalizing (1.43). For that, we begin by inverting the definitions:

$$\begin{cases} a_{\overrightarrow{\mathbf{k}}} = u^*_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} + v_{\overrightarrow{\mathbf{k}}} d^\dagger_{-\overrightarrow{\mathbf{k}}} \\ a^\dagger_{\overrightarrow{\mathbf{k}}} = u_{\overrightarrow{\mathbf{k}}} c^\dagger_{\overrightarrow{\mathbf{k}}} + v^*_{\overrightarrow{\mathbf{k}}} d_{-\overrightarrow{\mathbf{k}}} \end{cases} \qquad \begin{cases} b_{\overrightarrow{\mathbf{k}}} = u^*_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} + v_{\overrightarrow{\mathbf{k}}} c^\dagger_{-\overrightarrow{\mathbf{k}}} \\ b^\dagger_{\overrightarrow{\mathbf{k}}} = u_{\overrightarrow{\mathbf{k}}} d^\dagger_{\overrightarrow{\mathbf{k}}} + v^*_{\overrightarrow{\mathbf{k}}} c_{-\overrightarrow{\mathbf{k}}} \end{cases} \tag{1.46}$$

If we replace the expressions (1.46) into the Spin-Wave Hamiltonian (1.43), we get the following diagonal form [Appendix A.5]:

$$H_{SW} = 2Jzs \sum_{\overrightarrow{\mathbf{k}} \in FBZ_{sub}} \left[\sqrt{1 - \widetilde{\gamma}^2_{\overrightarrow{\mathbf{k}}}} \left\{ c^\dagger_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} + d^\dagger_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} + 1 \right\} \right] - JzNs$$

Apart from zero-point energy contributions, we get the two degenerate AFM magnon branches with the following dispersion relation:

$$\epsilon(\overrightarrow{\mathbf{k}}) = 2Jzs\sqrt{1 - \widetilde{\gamma}^2_{\overrightarrow{\mathbf{k}}}}, \quad \overrightarrow{\mathbf{k}} \in FBZ_{sub} \tag{1.47}$$

The ground-state energy is given as:

$$\epsilon_g = -JzNs(s+1) + 2JNzs \sum_{\overrightarrow{\mathbf{k}} \in FBZ_{sub}} \sqrt{1 - \widetilde{\gamma}^2_{\overrightarrow{\mathbf{k}}}}$$

As an important example, we can explicitly calculate the magnon dispersion relation for the case of an one-dimensional chain of spins (with a lattice parameter a). In this case, $z = 2$ and $\widetilde{\gamma}^{1D}_{\overrightarrow{\mathbf{k}}} = (1/z) \sum_{j \in viz} e^{-i\,\overrightarrow{\delta}_{\mathbf{j}} \cdot \overrightarrow{\mathbf{k}}} = 1/2 \left(e^{iak} + e^{-iak} \right) = \cos ak$, which leads to the following result:

$$\epsilon_{1D}(k) = 4Js\sqrt{1 - \cos^2 ak} = 4Js\,|\sin ak| \approx 4Jsa\,|k|\,, \quad k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a} \right] \tag{1.48}$$

The generalization for 2- and 3-dimensional cubic lattices is also trivial:

$$\widetilde{\gamma}^{2D}_{\mathbf{k}} = \frac{1}{2} \left\{ \cos(k_x a) + \cos(k_y a) \right\} \Rightarrow \epsilon_{2D}(\mathbf{k}) = 8Js\sqrt{1 - \frac{1}{4} \left\{ \cos(k_x a) + \cos(k_y a) \right\}^2} \sim 4\sqrt{2}Jsa \left| \overrightarrow{\mathbf{k}} \right| + ... \tag{1.49}$$

$$\begin{aligned} \widetilde{\gamma}^{3D}_{\mathbf{k}} &= \frac{1}{3} \left\{ \cos(k_x a) + \cos(k_y a) \right\} \Rightarrow \\ &\Rightarrow \epsilon_{3D}(\mathbf{k}) = 12Js\sqrt{1 - \frac{1}{9} \left\{ \cos(k_x a) + \cos(k_y a) + \cos(k_z a) \right\}^2} \sim 4\sqrt{3}Jsa \left| \overrightarrow{\mathbf{k}} \right| + ... \end{aligned} \tag{1.50}$$

As we can see, the AFM case yields a completely different low-energy spectra for the spin-wave excitations. They are also gapless, but with a linear dispersion relation, instead of a quadratic one.

1.3.3. Destruction of Neél Order By Quantum Fluctuations

With the new single-particle states, we can ask ourselves how close is the ground-state to a Neél State. For that, we calculate the $T = 0$ average of the staggered magnetization, i.e.:

$$S_{stagg} = \sum_{i\in\mathscr{L}_A} S_i^z - \sum_{j\in\mathscr{L}_B} S_j^z = Ns - \sum_{i\in\mathscr{L}_A} a_i^\dagger a_i - \sum_{j\in\mathscr{L}_B} b_j^\dagger b_j \tag{1.51}$$

Using the results in [Appendix A.5], we can rewrite (1.51) in momentum-space and in terms of the transformed operators c and d:

$$\begin{aligned} S_{stagg} &= Ns - \sum_{\mathbf{k}\in FBZ_{sub}} \left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\right) = \\ &= Ns - \sum_{\mathbf{k}\in FBZ_{sub}} \left[\left(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2\right)\left(c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}}\right) + 2u_{\mathbf{k}}v_{\mathbf{k}}\left(c_{\mathbf{k}}^\dagger d_{-\mathbf{k}}^\dagger + c_{\mathbf{k}} d_{-\mathbf{k}}\right) + 2v_{\mathbf{k}}^2\right] \end{aligned} \tag{1.52}$$

In Spin-Wave Theory, the ground-state is the vacuum of the c and d bosons. Therefore, at $T = 0K$, we have:

$$M_{Stagg}^z(T=0) = \lim_{N\to\infty}\left\{\frac{1}{Nv_{cell}}\langle\Omega|\, S_{stagg}\,|\Omega\rangle\right\} \tag{1.53}$$

$$\begin{aligned} &\frac{1}{Nv_{cell}}\langle\Omega|\, S_{stagg}\,|\Omega\rangle = \\ &= \frac{s}{v_{cell}} - \frac{1}{Nv_{cell}}\sum_{\mathbf{k}\in FBZ_{sub}} \langle\Omega|\left[\left(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2\right)\left(c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}}\right) + 2u_{\mathbf{k}}v_{\mathbf{k}}\left(c_{\mathbf{k}}^\dagger d_{-\mathbf{k}}^\dagger + c_{\mathbf{k}} d_{-\mathbf{k}}\right) + 2v_{\mathbf{k}}^2\right]|\Omega\rangle \\ &= \frac{s}{v_{cell}} - \frac{2}{Nv_{cell}}\sum_{\mathbf{k}\in FBZ_{sub}} v_{\mathbf{k}}^2 \underset{N\to\infty}{\longrightarrow} \frac{s}{v_{cell}} - \int_{\left[-\frac{\pi}{2a},\frac{\pi}{2a}\right]^d}\frac{d^d\mathbf{k}}{(2\pi)^d}\left\{\left(1-\widetilde{\gamma}_{\mathbf{k}}^2\right)^{-1/2} - 1\right\} \end{aligned} \tag{1.54}$$

In the hypercubic d-dimensional lattice, we can write a general formula for $\widetilde{\gamma}_{\mathbf{k}}$:

$$\widetilde{\gamma}_{\mathbf{k}} = \frac{1}{z}\sum_{j\in viz} e^{i\delta_j\cdot\mathbf{k}} = \frac{1}{d}\sum_{i=1}^{d}\cos(ak_i), \quad \text{where } k_i \quad \text{are the coordinates of } \overrightarrow{\mathbf{k}} \tag{1.55}$$

Since we are expecting to have 'IR divergent' corrections at low enough dimensions, we look only at the low-momenta behavior of the integrand in (1.54). In fact, the limit $|\mathbf{k}| \ll 1$ of the expression (1.55) is just $\widetilde{\gamma}_{\mathbf{k}} \approx 1 - \frac{a^2}{2d}|\mathbf{k}|^2 + ...$ Now, if we apply the latter approximation to the integrand in (1.54), we obtain the following expression:

$$\left(1-\widetilde{\gamma}_{\mathbf{k}}^2\right)^{-1/2} - 1 \approx \frac{1}{\sqrt{1-(1-\frac{a^2}{2d}|\mathbf{k}|^2)^2}} - 1 \approx \frac{\sqrt{d}}{a}\frac{1}{k} - 1 \approx \frac{\sqrt{d}}{a}\frac{1}{k} \tag{1.56}$$

Now, we can introduce a low-momentum cut-off — λ — and divide the integration (1.54) as:

$$\int_{\left[-\frac{\pi}{2a},\frac{\pi}{2a}\right]^d} = \int_{B(0,\lambda)} + \int_{\left[-\frac{\pi}{2a},\frac{\pi}{2a}\right]^d - B(0,\lambda)} \tag{1.57}$$

Finally, by using this separation, the correction to M^z_{Stagg} in (1.50) yields:

$$\begin{aligned}\int_{\left[-\frac{\pi}{2a},\frac{\pi}{2a}\right]^d} \frac{d^d\mathbf{k}}{(2\pi)^d}\left\{\left(1-\widetilde{\gamma}^2_{\mathbf{k}}\right)^{-1/2}-1\right\} &\approx \frac{\sqrt{d}}{(2\pi)^d a^2}\int_{B(0,\lambda)}\frac{d^d\mathbf{k}}{k} + \int_{\left[-\frac{\pi}{2a},\frac{\pi}{2a}\right]^d - B(0,\lambda)} \frac{d^d\mathbf{k}}{(2\pi)^d}\left\{\left(1-\widetilde{\gamma}^2_{\mathbf{k}}\right)^{-1/2}-1\right\} \\ &= \frac{\sqrt{d}S_{d-1}}{(2\pi)^d a^2}\int_{B(0,\lambda)} dk\, k^{d-2} + (\text{finite part})\end{aligned} \tag{1.58}$$

The expression (1.56) is divergent for $d = 1$, meaning that the Neél order is completely wiped out by the quantum fluctuations.[11] This result tells us that, although the Neél State can be used as a starting point for the study of the Heisenberg antiferromagnet lattices with $d > 1$, it is useless for treating the Heisenberg chain, since no traces of 'Neél-like character' are left in the exact ground-state. Therefore, to obtain information about the nature of the eigenstates in this case, one needs to take a quite different approach and develop an approximate theory that does not break the symmetry explicitly (as does the Holstein-Primakoff Spin-Wave Theory). This will be the subject of the whole Chapter 3.

1.3.4. Effect of Thermal Fluctuations

Finite temperature calculations can also be done to obtain the temperature dependence of the Neél Magnetization with temperature, for higher-dimensional lattices (like the 3-D cubic). That thermal correction can be written, using (1.54) and the expressions (A.22-23) of the [Appendix A.4], as follows:

$$M^z_{Stagg}(T,D) = M^z_{Stagg}(T=0,D) + \Delta M^z_{Stagg}(T,D)$$

With:

$$\begin{aligned}\Delta M^z_{Stagg}(T,D) &\sim -\frac{2}{N v_{cell}}\sum_{\overrightarrow{\mathbf{k}}\in FBZ_{sub}} \frac{1}{\sqrt{1-\widetilde{\gamma}^2_{\overrightarrow{\mathbf{k}}}}}\frac{1}{\exp(4Jsa\sqrt{D}\left|\overrightarrow{\mathbf{k}}\right|)-1} = \\ &= -\frac{S_{D-1}\sqrt{D}}{a(2\pi)^D}\int_0^{+\infty}\frac{dk k^{D-2}}{\exp(4\beta Jsa\sqrt{D}\left|\overrightarrow{\mathbf{k}}\right|)-1} = \begin{cases}\text{IR divergent} & \text{if } D=1,2\\ -\left(\frac{T}{T_C}\right)^2 & \text{if } D=3\end{cases}\end{aligned}$$

Once again, there is a complete destruction of the magnetic order for $D = 1$ and $D = 2$, which was already the case for the Ferromagnetic lattices.

[11] Notice that this divergence is independent of the spin multiplicity s. However, in the classical limit ($s \to \infty$) the Neél State is the true ground-state of H_{Heis}, the corrections due to magnons are irrelevant (i.e. 1st order in $1/s$). Unfortunately, the Universe doesn't seem to be very classical...

1.4. Spin-Waves in the Graphene Lattice

In this section, we will apply all the machinery of Spin-Wave Theory to calculate physical properties of the nearest-neighbor Heisenberg Model in the honeycomb lattice (which is a bipartite lattice). We will consider the FM, AFM and also the AFM with an easy-axis anisotropy.

1.4.1. The Ferromagnetic Model

1.4.1.1. Building the Spin-Wave Hamiltonian

The Hamiltonian for this model is given, as usual, by:

$$H = -\frac{J}{2}\sum_{\langle i,j\rangle} \vec{\mathbf{S}}(\vec{\mathbf{r}}_i)\cdot\vec{\mathbf{S}}(\vec{\mathbf{r}}_j); \quad \text{with } J>0 \tag{1.59}$$

Where $\vec{\mathbf{S}}(\vec{\mathbf{r}}_i)$ are local spin operators in the spin-s representation.

For a start, it is known that this system has the translation symmetry of an hexagonal Bravais lattice (with parameter a) containing a basis of two similar spins (A and B connected by a vector $\vec{\delta}$). In Figure 1.1, a section of that lattice is shown and a basis for the primitive translations is chosen — $\vec{\mathbf{a}}_1 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$ and $\vec{\mathbf{a}}_2 = -\frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$.

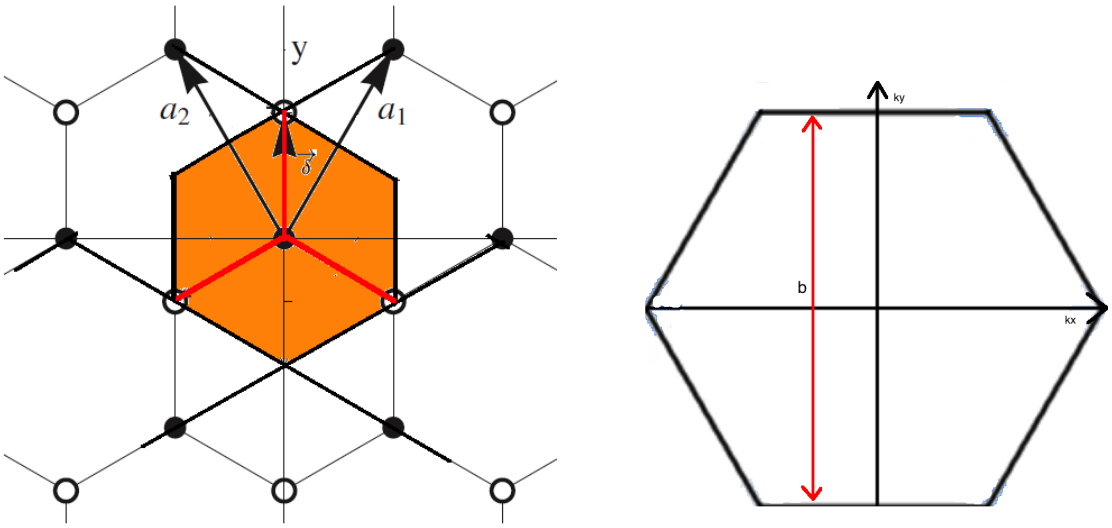


Figure 1.1.: Representation of a section of the Honeycomb Lattice. The A sites are represented by filled dots, while the B-sites are hollow. Drawn in the figure are: the Wigner-Seitz unit cell (in orange) for the underlying Bravais lattice, the ferromagnetic bonds (in red) and also the basis vectors chosen for representing the lattice translations. On the right, we have a picture of the corresponding First Brillouin Zone of the underlying Hexagonal Lattice (where $b = \frac{4\pi}{\sqrt{3}a}$).

As is also clear, the set of nearest-neighbors to an A-spin in the position $\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}$ are: the B-spins in his own unit cell and the B-spins of the cells centered at the positions $\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1$ and $\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2$.

This means that the Hamiltonian (1.59) can be written in terms of a single sum over the underlying hexagonal lattice $\mathscr{L}_{Hex}$:

$$H = -J \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \left\{ \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i + \vec{\delta}) + \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1 + \vec{\delta}) + \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2 + \vec{\delta}) \right\} \tag{1.60}$$

It is also convenient to write the interaction terms using ladder operators, i.e.:

$$\vec{\mathbf{S}}(\vec{\mathbf{r}}_1) \cdot \vec{\mathbf{S}}(\vec{\mathbf{r}}_2) = S^z(\vec{\mathbf{r}}_1) S^z(\vec{\mathbf{r}}_2) + 1/2 \left\{ S^+(\vec{\mathbf{r}}_1) S^-(\vec{\mathbf{r}}_2) + S^-(\vec{\mathbf{r}}_1) S^+(\vec{\mathbf{r}}_2) \right\} \tag{1.61}$$

Now, to find the Spin-Wave Hamiltonian associated with (1.60), one must introduce an Holstein-Primakoff representation for the spin operators at each site. Since the system is not a pure Bravais lattice, we must be careful and introduce different bosonic operators for each of the spins in a given cell. That is accomplished as follows:

$$S^z(\vec{\mathbf{R}}_i) = s - a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i), \quad S^+(\vec{\mathbf{R}}_i) = \sqrt{2s - a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i)}\, a(\vec{\mathbf{R}}_i), \quad S^-(\vec{\mathbf{R}}_i) = a^\dagger(\vec{\mathbf{R}}_i) \sqrt{2s - a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i)} \tag{1.62}$$

$$\begin{aligned} &S^z(\vec{\mathbf{R}}_i + \vec{\delta}) = s - b^\dagger(\vec{\mathbf{R}}_i) b(\vec{\mathbf{R}}_i), \quad S^+(\vec{\mathbf{R}}_i + \vec{\delta}) = \sqrt{2s - b^\dagger(\vec{\mathbf{R}}_i) b(\vec{\mathbf{R}}_i)}\, b(\vec{\mathbf{R}}_i), \\ &S^-(\vec{\mathbf{R}}_i + \vec{\delta}) = b^\dagger(\vec{\mathbf{R}}_i) \sqrt{2s - b^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i)} \end{aligned} \tag{1.63}$$

Where the operators a and b are bosonic Holstein-Primakoff (HP) operators that commute among them and with the operators in different cells.

The Spin-Wave approximation in (1.62) and (1.63) is done by expanding the square-roots to zeroth order in $1/s$. This yields the expressions $S^+(\vec{\mathbf{R}}_i) = a(\vec{\mathbf{R}}_i)\sqrt{2s} + ...$ *and* $S^-(\vec{\mathbf{R}}_i) = a^\dagger(\vec{\mathbf{R}}_i)\sqrt{2s} + ...$ for the raising/lowering spin operators (with analogous expressions for the B-spins). Plugging these expressions into the Hamiltonian (1.60), we get the following[12]:

$$\begin{aligned} H = -\frac{3Js^2N}{2} + Js \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \Big[& b^\dagger(\vec{\mathbf{R}}_i) b(\vec{\mathbf{R}}_i) + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + \\ & + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) + 3a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i) - a(\vec{\mathbf{R}}_i) \left\{ b^\dagger(\vec{\mathbf{R}}_i) + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + \right. \\ & \left. + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) \right\} - a^\dagger(\vec{\mathbf{R}}_i) \left\{ b(\vec{\mathbf{R}}_i) + b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) \right\} + \mathcal{O}(1/s) \Big] \end{aligned} \tag{1.64}$$

The Hamiltonian (1.64) is already the appropriate one for describing the Spin-Waves. It can simplified further, by going to the Fourier Space and take advantage of the translational symmetry of system. For that, we use the Lattice Fourier Transforms (LFT) of the HP operators defined in Section 1.2:

[12] N represents the total number of spins in the lattice, i.e. 2 per cell.

$$a(\vec{\mathbf{R}}_j) = \sqrt{2/N} \sum_{\vec{\mathbf{k}} \in FBZ} a_{\vec{\mathbf{k}}} e^{-i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \qquad a^\dagger(\vec{\mathbf{R}}_j) = \sqrt{2/N} \sum_{\vec{\mathbf{k}} \in FBZ} a^\dagger_{\vec{\mathbf{k}}} e^{i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \tag{1.65}$$

$$b(\vec{\mathbf{R}}_j) = \sqrt{2/N} \sum_{\vec{\mathbf{k}} \in FBZ} b_{\vec{\mathbf{k}}} e^{-i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \qquad b^\dagger(\vec{\mathbf{R}}_j) = \sqrt{2/N} \sum_{\vec{\mathbf{k}} \in FBZ} b^\dagger_{\vec{\mathbf{k}}} e^{i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \tag{1.66}$$

The corresponding inverse relations are:

$$a_{\vec{\mathbf{k}}} = \sqrt{2/N} \sum_{\vec{\mathbf{R}}_j \in \mathscr{L}_{Hex}} a(\vec{\mathbf{R}}_j) e^{i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \qquad a^\dagger_{\vec{\mathbf{k}}} = \sqrt{2/N} \sum_{\vec{\mathbf{R}}_j \in \mathscr{L}_{Hex}} a^\dagger(\vec{\mathbf{R}}_j) e^{-i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \tag{1.67}$$

$$b_{\vec{\mathbf{k}}} = \sqrt{2/N} \sum_{\vec{\mathbf{R}}_j \in \mathscr{L}_{Hex}} b(\vec{\mathbf{R}}_j) e^{i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \qquad b^\dagger_{\vec{\mathbf{k}}} = \sqrt{2/N} \sum_{\vec{\mathbf{R}}_j \in \mathscr{L}_{Hex}} b^\dagger(\vec{\mathbf{R}}_j) e^{-i\vec{\mathbf{R}}_j \cdot \vec{\mathbf{k}}} \tag{1.68}$$

Finally, we plug the definitions (1.65) and (1.66) into the Hamiltonian (1.64):

$$\begin{aligned} H_{SW} = 3Js \sum_{\vec{\mathbf{k}} \in FBZ} \Big[& b^\dagger_{\vec{\mathbf{k}}} b_{\vec{\mathbf{k}}} + a^\dagger_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} - 1/3 \left\{ 1 + e^{i\vec{\mathbf{a}}_1 \cdot \vec{\mathbf{k}}} + e^{i\vec{\mathbf{a}}_2 \cdot \vec{\mathbf{k}}} \right\} a_{\vec{\mathbf{k}}} b^\dagger_{\vec{\mathbf{k}}} - \\ & - 1/3 \left\{ 1 + e^{-i\vec{\mathbf{a}}_1 \cdot \vec{\mathbf{k}}} + e^{-i\vec{\mathbf{a}}_2 \cdot \vec{\mathbf{k}}} \right\} a^\dagger_{\vec{\mathbf{k}}} b_{\vec{\mathbf{k}}} \Big] \end{aligned}$$

Where the well known fact — $\sum_{\mathscr{L}} e^{i\vec{\mathbf{R}} \cdot (\vec{\mathbf{k}} - \vec{\mathbf{q}})} = \frac{N}{2} \delta_{\vec{\mathbf{k}}, \vec{\mathbf{q}}}$ — was used [Appendix A.1]. Now, we can define the gamma parameter for this problem as $\gamma_{\vec{\mathbf{k}}} = 1/3 \left\{ 1 + e^{i\vec{\mathbf{a}}_1 \cdot \vec{\mathbf{k}}} + e^{i\vec{\mathbf{a}}_2 \cdot \vec{\mathbf{k}}} \right\}$, and thus our Hamiltonian is seen to be quadratic, with a coupling between the a and b modes, given by the parameter $\gamma_{\vec{\mathbf{k}}}$. In matrix form, it is just:

$$H = -\frac{3Js^2 N}{2} + 3Js \sum_{\vec{\mathbf{k}} \in FBZ} \begin{bmatrix} a^\dagger_{\vec{\mathbf{k}}} & b^\dagger_{\vec{\mathbf{k}}} \end{bmatrix} \cdot \begin{bmatrix} 1 & -\gamma^*_{\vec{\mathbf{k}}} \\ -\gamma_{\vec{\mathbf{k}}} & 1 \end{bmatrix} \cdot \begin{bmatrix} a_{\vec{\mathbf{k}}} \\ b_{\vec{\mathbf{k}}} \end{bmatrix} \tag{1.69}$$

The Hamiltonian (1.69) is the one to be diagonalized in the next subsection.

1.4.1.2. Diagonalizing the Spin-Wave Hamiltonian

To diagonalize the quadratic form (1.69), we start by finding out what are the eigenvalues and corresponding eigenvectors of the matrix — $A = \begin{pmatrix} 1 & -\gamma^*_{\vec{\mathbf{k}}} \\ -\gamma_{\vec{\mathbf{k}}} & 1 \end{pmatrix}$. After writing the complex number $\gamma_{\vec{\mathbf{k}}}$ in the polar form — $\left|\gamma_{\vec{\mathbf{k}}}\right| e^{i\phi_{\vec{\mathbf{k}}}}$ — these are simply:

$$\begin{aligned} \lambda_1 &= 1 - \left|\gamma_{\vec{\mathbf{k}}}\right| \quad \rightarrow \left(e^{i\phi_{\vec{\mathbf{k}}}}, 1 \right) \\ \lambda_2 &= 1 + \left|\gamma_{\vec{\mathbf{k}}}\right| \quad \rightarrow \left(-e^{i\phi_{\vec{\mathbf{k}}}}, 1 \right) \end{aligned} \tag{1.70}$$

Hence, the coordinate transformation that diagonalizes (1.69) is given by:[13]

$$\begin{aligned} c_{\overrightarrow{\mathbf{k}}} &= 1/\sqrt{2}\left(e^{i\phi_{\overrightarrow{\mathbf{k}}}}a_{\overrightarrow{\mathbf{k}}} + b_{\overrightarrow{\mathbf{k}}}\right) \qquad & c^{\dagger}_{\overrightarrow{\mathbf{k}}} &= 1/\sqrt{2}\left(e^{-i\phi_{\overrightarrow{\mathbf{k}}}}a^{\dagger}_{\overrightarrow{\mathbf{k}}} + b^{\dagger}_{\overrightarrow{\mathbf{k}}}\right) \\ d_{\overrightarrow{\mathbf{k}}} &= 1/\sqrt{2}\left(-e^{i\phi_{\overrightarrow{\mathbf{k}}}}a_{\overrightarrow{\mathbf{k}}} + b_{\overrightarrow{\mathbf{k}}}\right) \qquad & d^{\dagger}_{\overrightarrow{\mathbf{k}}} &= 1/\sqrt{2}\left(-e^{-i\phi_{\overrightarrow{\mathbf{k}}}}a^{\dagger}_{\overrightarrow{\mathbf{k}}} + b^{\dagger}_{\overrightarrow{\mathbf{k}}}\right) \end{aligned} \tag{1.71}$$

Inverting the linear relations (1.71), we get:

$$\begin{aligned} a_{\overrightarrow{\mathbf{k}}} &= \frac{e^{-i\phi_{\overrightarrow{\mathbf{k}}}}}{\sqrt{2}}\left(c_{\overrightarrow{\mathbf{k}}} - d_{\overrightarrow{\mathbf{k}}}\right) \qquad & a^{\dagger}_{\overrightarrow{\mathbf{k}}} &= \frac{e^{i\phi_{\overrightarrow{\mathbf{k}}}}}{\sqrt{2}}\left(c^{\dagger}_{\overrightarrow{\mathbf{k}}} - d^{\dagger}_{\overrightarrow{\mathbf{k}}}\right) \\ b_{\overrightarrow{\mathbf{k}}} &= \frac{1}{\sqrt{2}}\left(c_{\overrightarrow{\mathbf{k}}} + d_{\overrightarrow{\mathbf{k}}}\right) \qquad & b^{\dagger}_{\overrightarrow{\mathbf{k}}} &= \frac{1}{\sqrt{2}}\left(c^{\dagger}_{\overrightarrow{\mathbf{k}}} + d^{\dagger}_{\overrightarrow{\mathbf{k}}}\right) \end{aligned} \tag{1.72}$$

Finally, we plug the relations (1.72) into the Hamiltonian (1.69), obtaining:

$$H = -\frac{3Js^2N}{2} + 3Js\sum_{\overrightarrow{\mathbf{k}}\in FBZ}\left\{\left(1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\right)c^{\dagger}_{\overrightarrow{\mathbf{k}}}c_{\overrightarrow{\mathbf{k}}} + \left(1 + \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\right)d^{\dagger}_{\overrightarrow{\mathbf{k}}}d_{\overrightarrow{\mathbf{k}}}\right\} = \tag{1.73}$$

$$= -\frac{3Js^2N}{2} + 3Js\sum_{\overrightarrow{\mathbf{k}}\in FBZ}\left\{\left(1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\right)n^{c}_{\overrightarrow{\mathbf{k}}} + \left(1 + \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\right)n^{d}_{\overrightarrow{\mathbf{k}}}\right\} \tag{1.74}$$

The above Hamiltonian is in diagonal form, and we see that, inside the Hexagonal First Brillouin Zone (FBZ) there are two branches for the spin-waves. This was expected since the number of degrees of freedom is twice the number of unit cells. The energies (or frequencies) are given by:

$$\begin{aligned} \epsilon_c(\overrightarrow{\mathbf{k}}) &= 3Js\left(1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\right) \\ \epsilon_d(\overrightarrow{\mathbf{k}}) &= 3Js\left(1 + \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\right) \end{aligned} \tag{1.75}$$

It is obvious that both of the Spin-Wave branches represent deviations that increase the overall energy of the system, since $\left|\gamma_{\overrightarrow{\mathbf{k}}}\right| = 1/3\left|1 + e^{-i\overrightarrow{\mathbf{a}}_1\cdot\overrightarrow{\mathbf{k}}} + e^{-i\overrightarrow{\mathbf{a}}_2\cdot\overrightarrow{\mathbf{k}}}\right| \leq 1$. This is a reassuring fact, because we know that the fully magnetized state is an exact ground-state for the system. Furthermore, only the C-branch contains gapless states (because $\epsilon_d(\overrightarrow{\mathbf{k}}) \geq 1$) which means that only the C-branch will contribute to the physics of the system, at low temperatures.

1.4.1.3. The Spin-Wave Dispersion Relation

Equations (1.75) give us the Spin-Wave dispersion relations in the Hexagonal Lattice's First Brillouin Zone. But, before plotting them, we can start by seeing what is the asymptotic behavior of the C-branch near the Γ-point (where it attains the minimum value and there is no gap.). This can be done by expanding $\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|$ up to second order in ak_x and ak_y, i.e.:

$$\gamma_{\overrightarrow{\mathbf{k}}} = 1/3\left|1 + e^{-i\overrightarrow{\mathbf{a}}_1\cdot\overrightarrow{\mathbf{k}}} + e^{-i\overrightarrow{\mathbf{a}}_2\cdot\overrightarrow{\mathbf{k}}}\right| \simeq 1 - i\frac{a}{\sqrt{3}}k_y - \frac{a^2}{4}\left(\frac{k_x^2}{3} + k_y^2\right) + ... \tag{1.76}$$

[13] Note that the factors of $1/\sqrt{2}$ are put in, to ensure the correct normalization of the commutators between the new bosonic operators.

Equation (1.76) means that the modulus of $\gamma_{\overrightarrow{\mathbf{k}}}$ can be expanded as:

$$\left|\gamma_{\overrightarrow{\mathbf{k}}}\right| = \sqrt{(1 - \frac{a^2}{4}\left(\frac{k_x^2}{3} + k_y^2\right))^2 + \frac{a^2 k_y^2}{3}} \simeq 1 - \frac{a^2}{12}\left(k_x^2 + k_y^2\right) + ... \tag{1.77}$$

Yielding a gapless quadratic behavior for the C-branch dispersion relation:

$$\epsilon_c(\overrightarrow{\mathbf{k}}) \simeq \frac{Jsa^2}{4}\left[k_x^2 + k_y^2\right] + ... = \frac{Jsa^2}{4}\left|\overrightarrow{\mathbf{k}}\right|^2 + ... \tag{1.78}$$

Since the the D-branch of the Spin-Waves is frozen at low temperatures, we can then say that the qualitative behavior of this model is exactly the same as the one expected for an isotropic FM in a square lattice.

We conclude this discussion by showing the plots of the obtained dispersion relations on the Figure 1.2.

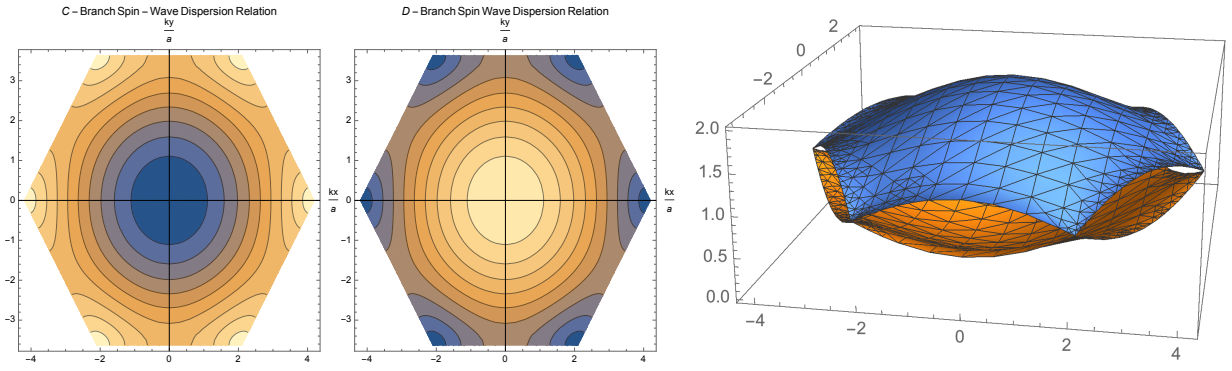


Figure 1.2.: On the left side, we have the contour plots of the functions $\epsilon_c(\overrightarrow{\mathbf{k}})$ and $\epsilon_d(\overrightarrow{\mathbf{k}})$, while on the right we represented a profile 3-D plot of both branches. All the plots are done in the First Brillouin Zone of the Hexagonal Lattice.

1.4.1.4. Spin-Spin Correlation Function and Interpretation of the Spin-Wave Branches

We obtained the spectrum for the spin-waves in this system, but we still need to interpret what kind of spin deviations are represented by each of the branches. We can start by calculating the correlation functions between the two spins in each hexagonal cell, for a state with one magnon of each type (and crystal-momentum $\overrightarrow{\mathbf{k}}$). I.e.:

$$C_{AB}^c(\overrightarrow{\mathbf{k}}, \overrightarrow{\mathbf{R}}_i) = \left\langle n_{\overrightarrow{\mathbf{k}}}^c = 1, 0... \right| \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i) \cdot \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i + \overrightarrow{\delta}) \left| n_{\overrightarrow{\mathbf{k}}}^c = 1, 0... \right\rangle - s^2 \tag{1.79}$$

$$C_{AB}^d(\overrightarrow{\mathbf{k}}, \overrightarrow{\mathbf{R}}_i) = \left\langle n_{\overrightarrow{\mathbf{k}}}^d = 1, 0... \right| \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i) \cdot \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i + \overrightarrow{\delta}) \left| n_{\overrightarrow{\mathbf{k}}}^d = 1, 0... \right\rangle - s^2 \tag{1.80}$$

The states over which we take averages are simply — $\left|n_{\overrightarrow{\mathbf{k}}}^c = 1, 0...\right\rangle = c_{\overrightarrow{\mathbf{k}}}^\dagger \left|0\right\rangle$ and $\left|n_{\overrightarrow{\mathbf{k}}}^d = 1, 0...\right\rangle = d_{\overrightarrow{\mathbf{k}}}^\dagger \left|0\right\rangle$. As was done before, both Equations (1.79) and (1.80) can be written in terms of Holstein-Primakoff operators, in the Spin-Wave approximation, yielding:

$$C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=\left\langle S^z(\overrightarrow{\mathbf{R}}_i)S^z(\overrightarrow{\mathbf{R}}_i+\overrightarrow{\delta})+1/2\left\{S^+(\overrightarrow{\mathbf{R}}_i)S^-(\overrightarrow{\mathbf{R}}_i+\overrightarrow{\delta})+S^-(\overrightarrow{\mathbf{R}}_i)S^+(\overrightarrow{\mathbf{R}}_i+\overrightarrow{\delta})\right\}\right\rangle-s^2= \tag{1.81}$$

$$=s\left\langle b^\dagger(\overrightarrow{\mathbf{R}}_i)a(\overrightarrow{\mathbf{R}}_i)+b^\dagger(\overrightarrow{\mathbf{R}}_i)a(\overrightarrow{\mathbf{R}}_i)-a^\dagger(\overrightarrow{\mathbf{R}}_i)a(\overrightarrow{\mathbf{R}}_i)-b^\dagger(\overrightarrow{\mathbf{R}}_i)b(\overrightarrow{\mathbf{R}}_i)\right\rangle$$

Using the definitions (1.65) and (1.66), we can rewrite (1.81) in momentum-space:

$$C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=\frac{2s}{N}\sum_{\overrightarrow{\mathbf{q}}\,\overrightarrow{\mathbf{p}}\in FBZ}\left\langle b^\dagger_{\overrightarrow{\mathbf{p}}}a_{\overrightarrow{\mathbf{q}}}+a^\dagger_{\overrightarrow{\mathbf{p}}}b_{\overrightarrow{\mathbf{q}}}-a^\dagger_{\overrightarrow{\mathbf{p}}}a_{\overrightarrow{\mathbf{q}}}-b^\dagger_{\overrightarrow{\mathbf{p}}}b_{\overrightarrow{\mathbf{q}}}\right\rangle e^{i\overrightarrow{\mathbf{R_i}}\cdot(\overrightarrow{\mathbf{p}}-\overrightarrow{\mathbf{q}})} \tag{1.82}$$

The above expression involves a double sum over the FBZ of the Hexagonal Lattice, however by using the lattice symmetry, we can argue that $C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)$ must be independent of the lattice vector $\overrightarrow{\mathbf{R}}_i$. This means that:

$$C_{AB}(\overrightarrow{\mathbf{k}})\equiv\frac{2}{N}\sum_{\overrightarrow{\mathbf{R}}_i\in\mathscr{L}_{Hex}}C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=\frac{2s}{N}\sum_{\overrightarrow{\mathbf{q}}\in FBZ}\left\langle b^\dagger_{\overrightarrow{\mathbf{q}}}a_{\overrightarrow{\mathbf{q}}}+a^\dagger_{\overrightarrow{\mathbf{q}}}b_{\overrightarrow{\mathbf{q}}}-a^\dagger_{\overrightarrow{\mathbf{q}}}a_{\overrightarrow{\mathbf{q}}}-b^\dagger_{\overrightarrow{\mathbf{q}}}b_{\overrightarrow{\mathbf{q}}}\right\rangle \tag{1.83}$$

Finally, we replace the a's and b's in (1.83) by the normal mode operators, using (1.72). We get then:

$$C_{AB}(\overrightarrow{\mathbf{k}})=-\frac{2s}{N}\sum_{\overrightarrow{\mathbf{k}}\in FBZ}\left\langle\left(1-\cos(\phi_{\overrightarrow{\mathbf{k}}})\right)c^\dagger_{\overrightarrow{\mathbf{k}}}c_{\overrightarrow{\mathbf{k}}}+\left(1+\cos(\phi_{\overrightarrow{\mathbf{k}}})\right)d^\dagger_{\overrightarrow{\mathbf{k}}}d_{\overrightarrow{\mathbf{k}}}+\right.$$
$$\left.+i\sin\left(\phi_{\overrightarrow{\mathbf{k}}}\right)\left\{c^\dagger_{\overrightarrow{\mathbf{k}}}d_{\overrightarrow{\mathbf{k}}}-d^\dagger_{\overrightarrow{\mathbf{k}}}c_{\overrightarrow{\mathbf{k}}}\right\}\right\rangle \tag{1.84}$$

From (1.84), we can calculate the correlation functions defined in (1.79) and (1.80) very easily:

$$C^c_{AB}(\overrightarrow{\mathbf{k}})=-\frac{2s}{N}\left(1-\cos(\phi_{\overrightarrow{\mathbf{k}}})\right),\quad C^d_{AB}(\overrightarrow{\mathbf{k}})=-\frac{2s}{N}\left(1+\cos(\phi_{\overrightarrow{\mathbf{k}}})\right) \tag{1.85}$$

Where $\phi_{\overrightarrow{\mathbf{k}}}$ is the phase of the parameter $\gamma_{\overrightarrow{\mathbf{k}}}$. It can be expressed as follows:

$$\phi_{\overrightarrow{\mathbf{k}}}=\arctan\left[\frac{\sin\left(\overrightarrow{\mathbf{k}}\cdot\overrightarrow{\mathbf{a}}_1\right)+\sin\left(\overrightarrow{\mathbf{k}}\cdot\overrightarrow{\mathbf{a}}_2\right)}{1+\cos\left(\overrightarrow{\mathbf{k}}\cdot\overrightarrow{\mathbf{a}}_1\right)+\cos\left(\overrightarrow{\mathbf{k}}\cdot\overrightarrow{\mathbf{a}}_2\right)}\right]\approx\frac{\overrightarrow{\mathbf{k}}\cdot(\overrightarrow{\mathbf{a}}_1+\overrightarrow{\mathbf{a}}_2)}{3}+\mathcal{O}((ka)^2)=\frac{k_ya}{\sqrt{3}} \tag{1.86}$$

Where we took the long-wavelength limit. The plots of the two correlation functions (1.85) are given in Figure 1.3, over the FBZ of the underlying hexagonal lattice.

To get an intuitive feeling about the shape of the deviations represented by these modes, it is interesting to analyze the low-$\left|\overrightarrow{\mathbf{k}}\right|$ behavior of the expressions (1.85). This yields the following:

$$C^c_{AB}(\overrightarrow{\mathbf{k}})=-\frac{sa^2k_y^2}{3N}+\mathcal{O}((ka)^4),\quad C^d_{AB}(\overrightarrow{\mathbf{k}})=-\frac{4s}{N}+\frac{sa^2k_y^2}{3N}+\mathcal{O}((ka)^4) \tag{1.87}$$

The results (1.87) strongly support the interpretation of the C-Branch as an **Acoustic Spin-Wave**, in which the spins on each unit cell are aligned with each other, but there is a modulation along the crystal. The D-Branch, on the other hand, is an **Optical Spin-Wave**, where (even at $\vec{\mathbf{k}} \to 0$), the spins inside each cell are out of alignment by an amount which scales as $1/N$ (but grows linearly with the occupation number of D-bosons.):

$$\left\langle n^c_{\vec{\mathbf{k}}} = 1, 0... \right| \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i + \vec{\delta}) \left| n^c_{\vec{\mathbf{k}}} = 1, 0... \right\rangle \underset{\vec{\mathbf{k}} \to 0}{\to} s^2 + ... \tag{1.88}$$

$$\left\langle n^d_{\vec{\mathbf{k}}} = 1, 0... \right| \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i + \vec{\delta}) \left| n^d_{\vec{\mathbf{k}}} = 1, 0... \right\rangle \underset{\vec{\mathbf{k}} \to 0}{\to} s(s - \frac{4}{N}) + ... \tag{1.89}$$

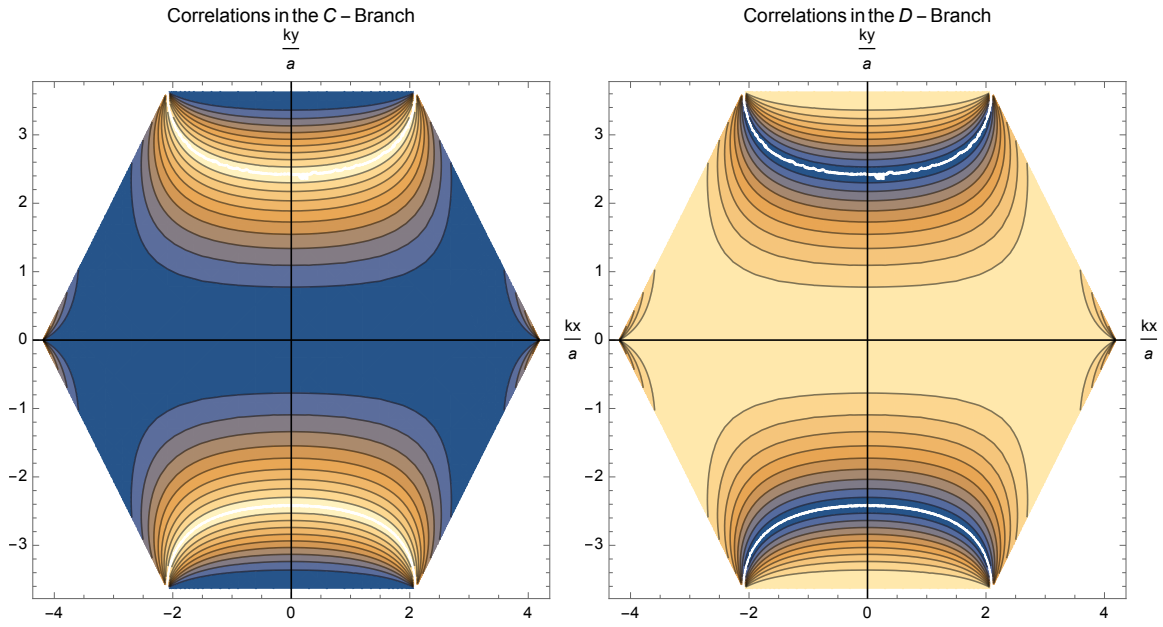


Figure 1.3.: On the very left, we represent a contour plot of C^c_{AB} and at the right, we have the corresponding plot for C^d_{AB}. As can be seen, the interpretation given approximately at (1.88) and (1.89) is valid in a relatively wide region of the FBZ.

1.4.1.5. Finite Temperature Properties

Using the above results, we can also calculate the effect of low-energy spin-waves in the magnetization of the system. In other words, we wish to calculate the following average over an equilibrium thermal state:

$$M^z(T) = \frac{2}{N v_{cell}} \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \left\langle S^z(\vec{\mathbf{R}}_i) + S^z(\vec{\mathbf{R}}_i + \vec{\delta}) \right\rangle_T = \tag{1.90}$$

$$= M_0 \left\{ 1 - \frac{1}{Ns} \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \left\langle a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i) + b^\dagger(\vec{\mathbf{R}}_i) b(\vec{\mathbf{R}}_i) \right\rangle_T \right\}$$

Where $M_0 = \frac{2s}{v_{cell}}$ is the expected magnetization at $T = 0K$. Expressing everything in terms of the normal mode operators, we get:

$$M^z(T) = M_0 \left\{ 1 - \frac{1}{Ns} \sum_{\vec{\mathbf{k}} \in FBZ} \left(\left\langle n^c_{\vec{\mathbf{k}}} \right\rangle_T + \left\langle n^d_{\vec{\mathbf{k}}} \right\rangle_T \right) \right\} \tag{1.91}$$

In equilibrium, we know that the average occupation numbers for each of the modes is given by the Planck Distribution — $B(\epsilon, T) = \frac{1}{e^{\epsilon/k_B T} - 1}$. Therefore (1.91) becomes the following, in the thermodynamic limit:

$$M^z(T) = M_0 \left\{ 1 - \frac{v_{cell}}{8\pi^2 s} \int_{FBZ} d^2\vec{\mathbf{k}} \left[\frac{1}{e^{3Js/k_B T(1-|\gamma_{\vec{\mathbf{k}}}|)} - 1} + \frac{1}{e^{3Js/k_B T(1+|\gamma_{\vec{\mathbf{k}}}|)} - 1} \right] \right\} \tag{1.92}$$

Obviously, since the D-branch of Spin-Waves has a gap over the ground-state (of energy $3Js$), it is reasonable to discard the last term, as long as $T \ll \frac{3Js}{k_B}$. In that same regime, the greatest contribution to the magnetization will come from the C-modes that are closer to the Γ-point and we can safely use the quadratic approximation for the dispersion relation. Finally, we can write:

$$M^z(T) = M_0 \left\{ 1 - \frac{v_{cell}}{4\pi s} \int_0^{\Lambda} dk \left[\frac{k}{e^{Jsa^2k^2/4k_B T} - 1} \right] \right\} \tag{1.93}$$

Which depends on an arbitrarily chosen momentum cut-off Λ. To calculate (1.93), we need to adimensionalize the integral, by choosing the variable $u = \frac{k}{\Lambda}$:

$$\frac{\Delta M^z}{M_0} = -\frac{v_{cell}\Lambda^2}{4\pi s} \int_0^1 du \left[\frac{u}{e^{Jsa^2\Lambda^2u^2/4k_B T} - 1} \right] \to -\infty \tag{1.94}$$

As will be seen in the next chapter, this divergence is the expected consequence of the **Mermin-Wagner Theorem** for lattice spin models, with finite-ranged interactions.

Therefore, all the derivation of the Spin-Wave Spectrum for this model is rendered useless in any finite temperature calculation, since it assumes the existence of a spontaneous magnetization that is not real for $T > 0$.

1.4.2. The Antiferromagnetic Model

1.4.2.1. Building the Spin-Wave Hamiltonian

For treating the AFM case, we start by the following Hamiltonian:

$$H = J \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \left\{ \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i + \vec{\delta}) + \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1 + \vec{\delta}) + \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2 + \vec{\delta}) \right\} \tag{1.95}$$

With $J > 0$. Since the lattice is bipartite, we can assume a Néel state (1.96) as a starting point for the $1/s$ expansion.

$$|\Psi_{N\acute{e}el}\rangle = \otimes_{i\in\mathscr{L}_A}\left\{\left|\vec{\mathbf{R}}_i, s, s\right\rangle \otimes \left|\vec{\mathbf{R}}_i + \vec{\delta}, s, -s\right\rangle\right\} \tag{1.96}$$

To do the expansion around $|\Psi_{N\acute{e}el}\rangle$, we represent the spin operators using Holstein-Primakoff bosons, as explained in the Section 1.2. This yields:

$$\begin{aligned} S^z(\vec{\mathbf{R}}_i) &= s - a^\dagger(\vec{\mathbf{R}}_i)a(\vec{\mathbf{R}}_i), \quad S_i^+(\vec{\mathbf{R}}_i) \approx \sqrt{2s}\, a(\vec{\mathbf{R}}_i), \quad S^-(\vec{\mathbf{R}}_i) \approx \sqrt{2s}\, a^\dagger(\vec{\mathbf{R}}_i) \\ &, \\ S^z(\vec{\mathbf{R}}_i + \vec{\delta}) &= -s + b^\dagger(\vec{\mathbf{R}}_i)b(\vec{\mathbf{R}}_i), \quad S^-(\vec{\mathbf{R}}_i + \vec{\delta}) \approx -\sqrt{2s}\, b(\vec{\mathbf{R}}_i), \quad S^+(\vec{\mathbf{R}}_i + \vec{\delta}) \simeq -\sqrt{2s}\, b^\dagger(\vec{\mathbf{R}}_i) \end{aligned} \tag{1.97}$$

By replacing the definitions (1.97) into the Hamiltonian (1.95), we get the effective Spin-Wave Hamiltonian for the AFM model:

$$\begin{aligned} H = -\frac{3Js^2N}{2} + Js \sum_{\vec{\mathbf{R}}_i\in\mathscr{L}_{Hex}} \Big[& b^\dagger(\vec{\mathbf{R}}_i)b(\vec{\mathbf{R}}_i) + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1)b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + \\ & + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2)b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) + 3a^\dagger(\vec{\mathbf{R}}_i)a(\vec{\mathbf{R}}_i) - a^\dagger(\vec{\mathbf{R}}_i)\Big\{b^\dagger(\vec{\mathbf{R}}_i) + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + \\ & + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2)\Big\} - a(\vec{\mathbf{R}}_i)\Big\{b(\vec{\mathbf{R}}_i) + b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2)\Big\} + \mathcal{O}(1/s)\Big] \end{aligned} \tag{1.98}$$

The Hamiltonian (1.98) can be rewritten in momentum-space using (1.65) and (1.66), and takes the form:

$$H = -\frac{3Js^2N}{2} + 3Js \sum_{\vec{\mathbf{k}}\in FBZ} \left[b^\dagger_{-\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}} + a^\dagger_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} - \gamma^*_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}} b^\dagger_{-\vec{\mathbf{k}}} - \gamma_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}}\right] \tag{1.99}$$

As expected, (1.99) is very different from the FM one and does not conserve the number of particles (i.e. it does not have global gauge symmetry).

1.4.2.2. Diagonalizing the Hamiltonian

Diagonalizing the above Hamiltonian involves finding a Bogoliubov-Valatin Transformation that eliminates the anomalous terms. This transformation goes as follows:

$$\begin{cases} c_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} e^{-i\phi_{\vec{\mathbf{k}}}} b^\dagger_{-\mathbf{k}} \\ c^\dagger_{\mathbf{k}} = u_{\mathbf{k}} a^\dagger_{\mathbf{k}} - v_{\mathbf{k}} e^{i\phi_{\vec{\mathbf{k}}}} b_{-\mathbf{k}} \end{cases} \qquad \begin{cases} d_{\mathbf{k}} = u_{\mathbf{k}} e^{i\phi_{\vec{\mathbf{k}}}} b_{-\mathbf{k}} - v_{\mathbf{k}} a^\dagger_{\mathbf{k}} \\ d^\dagger_{\mathbf{k}} = u_{\mathbf{k}} e^{-i\phi_{\vec{\mathbf{k}}}} b^\dagger_{-\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}} \end{cases} \tag{1.100}$$

Where $u_{\overrightarrow{\mathbf{k}}}$ and $v_{\overrightarrow{\mathbf{k}}}$ are assumed real numbers[14]. This transformation must preserve the fact that $c_{\overrightarrow{\mathbf{k}}}$ and $d_{\overrightarrow{\mathbf{k}}}$ represent independent bosonic degrees of freedom. So:

$$\left[c_{\overrightarrow{\mathbf{k}}}, c^{\dagger}_{\overrightarrow{\mathbf{k}}}\right] = u^2_{\overrightarrow{\mathbf{k}}} - v^2_{\overrightarrow{\mathbf{k}}} = 1$$

We can then invert the tranformation (1.100) and parametrize it, using $u_{\overrightarrow{\mathbf{k}}} = \cosh\eta_{\mathbf{k}}$ and $v_{\overrightarrow{\mathbf{k}}} = \sinh\eta_{\mathbf{k}}$:

$$\begin{cases} a_{\overrightarrow{\mathbf{k}}} = \cosh\eta_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} + \sinh\eta_{\overrightarrow{\mathbf{k}}} d^{\dagger}_{\overrightarrow{\mathbf{k}}} \\ a^{\dagger}_{\overrightarrow{\mathbf{k}}} = \cosh\eta_{\overrightarrow{\mathbf{k}}} c^{\dagger}_{\overrightarrow{\mathbf{k}}} + \sinh\eta_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} \end{cases} \qquad \begin{cases} b_{-\overrightarrow{\mathbf{k}}} = e^{-i\phi_{\overrightarrow{\mathbf{k}}}} \cosh\eta_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} + e^{-i\phi_{\overrightarrow{\mathbf{k}}}} \sinh\eta_{\overrightarrow{\mathbf{k}}} c^{\dagger}_{\overrightarrow{\mathbf{k}}} \\ b^{\dagger}_{-\overrightarrow{\mathbf{k}}} = e^{i\phi_{\overrightarrow{\mathbf{k}}}} \cosh\eta_{\overrightarrow{\mathbf{k}}} d^{\dagger}_{\overrightarrow{\mathbf{k}}} + e^{i\phi_{\overrightarrow{\mathbf{k}}}} \sinh\eta_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} \end{cases} \tag{1.101}$$

Replacing the above definitions into the Hamiltonian (1.99) yields the following result:

$$\begin{aligned} H = -\frac{3Js^2N}{2} + 3Js \sum_{\overrightarrow{\mathbf{k}}\in FBZ} \Bigg[& 2\left|\gamma_{\overrightarrow{\mathbf{k}}}\right| \cosh\eta_{\overrightarrow{\mathbf{k}}} \sinh\eta_{\overrightarrow{\mathbf{k}}} + 2\sinh^2\eta_{\overrightarrow{\mathbf{k}}} + \\ & + \left\{c^{\dagger}_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} + d^{\dagger}_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}}\right\} \left\{\sinh^2\eta_{\overrightarrow{\mathbf{k}}} + \cosh^2\eta_{\overrightarrow{\mathbf{k}}} - 2\left|\gamma_{\overrightarrow{\mathbf{k}}}\right| \cosh\eta_{\overrightarrow{\mathbf{k}}} \sinh\eta_{\overrightarrow{\mathbf{k}}}\right\} - \\ & - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right| \left\{c_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} + c^{\dagger}_{\overrightarrow{\mathbf{k}}} d^{\dagger}_{\overrightarrow{\mathbf{k}}}\right\} \left\{\sinh^2\eta_{\overrightarrow{\mathbf{k}}} + \cosh^2\eta_{\overrightarrow{\mathbf{k}}} - \frac{2}{\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|} \cosh\eta_{\overrightarrow{\mathbf{k}}} \sinh\eta_{\overrightarrow{\mathbf{k}}}\right\} \Bigg] \end{aligned} \tag{1.102}$$

From the ugly expression (1.102), the anomalous terms — $c_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} + c^{\dagger}_{\overrightarrow{\mathbf{k}}} d^{\dagger}_{\overrightarrow{\mathbf{k}}}$ — are eliminated by choosing $\eta_{\overrightarrow{\mathbf{k}}}$ as one solution of the following equation:

$$\sinh^2\eta_{\overrightarrow{\mathbf{k}}} + \cosh^2\eta_{\overrightarrow{\mathbf{k}}} - \frac{2}{\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|} \cosh\eta_{\overrightarrow{\mathbf{k}}} \sinh\eta_{\overrightarrow{\mathbf{k}}} = 0 \Leftrightarrow 2x^2 - 1 = \frac{2x}{\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|}\sqrt{x^2-1} \tag{1.103}$$

By squaring the last equation (where $x \geq 1$, by definition), one gets the biquadratic equation — $x^4 - x^2 + \frac{\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}{4\left(\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2 - 1\right)} = 0$, whose solutions are:

$$x = \sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}} \geq 1 \tag{1.104}$$

Or, in terms of the original variables:

$$\begin{aligned} \cosh\eta_{\overrightarrow{\mathbf{k}}} &= \sqrt{\tfrac{1}{2}\sqrt{\tfrac{1}{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}} + \tfrac{1}{2}} \\ \sinh\eta_{\overrightarrow{\mathbf{k}}} &= \sqrt{\tfrac{1}{2}\sqrt{\tfrac{1}{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}} - \tfrac{1}{2}} \end{aligned} \tag{1.105}$$

[14]Note that, contrarily to the cases treated in Section 1.3., the parameter $\gamma_{\overrightarrow{\mathbf{k}}}$ is not real, so a phase $\phi_{\overrightarrow{\mathbf{k}}}$ is needed to find a suitable Bogoliubov-Valatin Transformation.

Plugging the expressions (1.105) into (1.102), we arrive at a diagonal Hamiltonian:

$$H = -\frac{3Js(s+1)N}{2} + 3Js \sum_{\overrightarrow{\mathbf{k}} \in FBZ} \left[\left\{ \sqrt{1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2} \right\} \left(c^{\dagger}_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} + d^{\dagger}_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} \right) \right] + 3Js \sum_{\overrightarrow{\mathbf{k}} \in FBZ} \sqrt{1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2} \tag{1.106}$$

1.4.2.3. Corrections to the Ground-State Energy and the Spin-Wave Dispersion Relation

Since the Néel State is not the true ground-state for the model, the vacuum energy of the diagonalized Hamiltonian is actually lower than the average energy of $|\Psi_{Néel}\rangle$[15]. Hence, the correction to the ground-state energy can be written (in the thermodynamic limit), as follows:

$$\Delta\epsilon_{GS} = -\frac{3NJs}{2} \left\{ 1 - \frac{v_{cell}}{4\pi^2} \int_{FBZ} d^2\overrightarrow{\mathbf{k}} \sqrt{1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2} \right\} \tag{1.107}$$

From the previous FM calculation, we know that the parameter $\gamma_{\overrightarrow{\mathbf{k}}}$ has the following modulus:

$$\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2 = {}^1\!/_9 \left(\left[1 + \cos\left(\frac{k_x a}{2} + \frac{\sqrt{3}k_y a}{2} \right) + \cos\left(\frac{k_x a}{2} - \frac{\sqrt{3}k_y a}{2} \right) \right]^2 + \left[\sin\left(-\frac{k_x a}{2} - \frac{\sqrt{3}k_y a}{2} \right) + \sin\left(\frac{k_x a}{2} - \frac{\sqrt{3}k_y a}{2} \right) \right]^2 \right) \tag{1.108}$$

Hence, the dimensionless version of the integral in (1.107) is $\frac{v_{cell}}{4\pi^2} \int_{FBZ} d^2\overrightarrow{\mathbf{k}} = \frac{v_{cell}}{4a^2\pi^2} \int_{FBZ(a=1)} dxdy$. By numerical integration over the Hexagonal FBZ, we got the following value:

$$\frac{v_{cell}}{4\pi^2} \int_{FBZ} d^2\overrightarrow{\mathbf{k}} \sqrt{1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2} = 0.9124 \frac{v_{cell}}{a^2} = 0.7902 \tag{1.109}$$

Which means that: $\Delta\epsilon_{GS} \simeq -0.3148 \times NJs$.

Besides this correction, equation (1.106) also give us two degenerate gapless Spin-Wave Modes, whose dispersion relation is given by (1.110) and plotted in Figure 1.4.

$$\epsilon^c_{AFM}(\overrightarrow{\mathbf{k}}) = \epsilon^d_{AFM}(\overrightarrow{\mathbf{k}}) = 3Js\sqrt{1 - \left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2} \tag{1.110}$$

Unlike the FM case, the two branches are linear (dispersionless modes) for the area near the Γ-point. Plugging the approximate expression — $\left|\gamma_{\overrightarrow{\mathbf{k}}}\right| \simeq 1 - \frac{a^2}{12}\left(k_x^2 + k_y^2\right) + ...$ — and expanding till the first non-zero order, we arrive exactly at that conclusion:

$$\epsilon^c_{AFM}(\overrightarrow{\mathbf{k}}) = \epsilon^d_{AFM}(\overrightarrow{\mathbf{k}}) \simeq 3Js\sqrt{\frac{a^2}{6}\left|\overrightarrow{\mathbf{k}}\right|^2 + ...} = \frac{3Jsa}{\sqrt{6}}\left|\overrightarrow{\mathbf{k}}\right| + ... \tag{1.111}$$

[15] Looking at the bound (1.14), the minimum value possible for this energy would be $-{}^3\!/_2 Js(s+1)N$. However, the zero-point motion acts to increase the actual eigenenergy of the ground-state.

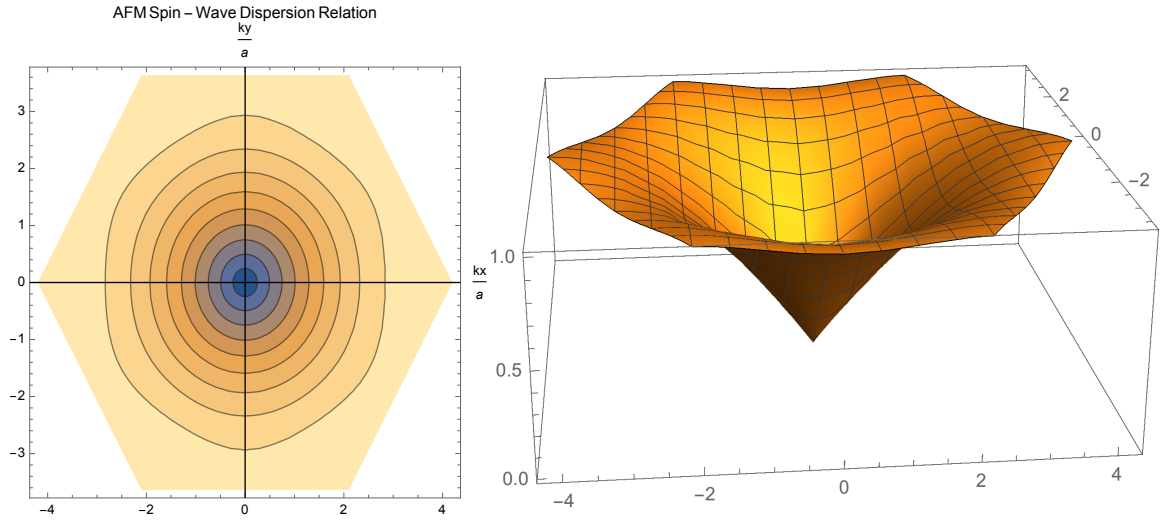


Figure 1.4.: On the left side, we have the contour plot of the functions $\epsilon^c_{AFM}(\overrightarrow{\mathbf{k}})$ and $\epsilon^d_{AFM}(\overrightarrow{\mathbf{k}})$, which are the same, in this case. On the right, we represented a profile 3-D plot of both branches. All the plots are done in the First Brillouin Zone of the Hexagonal Lattice.

1.4.2.4. Correlation Functions and Interpretation of the Spin-Wave Modes

Now, we wish to calculate the spin-spin correlation functions between neighboring spins, for a state containing one spin-wave quantum of each kind, i.e.:

$$C^c_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=\left\langle n^c_{\overrightarrow{\mathbf{k}}}=1,0...\right|\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i)\cdot\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i+\overrightarrow{\delta})\left|n^c_{\overrightarrow{\mathbf{k}}}=1,0...\right\rangle+s^2 \tag{1.112}$$

$$C^d_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=\left\langle n^d_{\overrightarrow{\mathbf{k}}}=1,0...\right|\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i)\cdot\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i+\overrightarrow{\delta})\left|n^d_{\overrightarrow{\mathbf{k}}}=1,0...\right\rangle+s^2 \tag{1.113}$$

Once again, the above functions can be written in terms of the a and b HP operators, yielding:

$$C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=s\left\langle a^\dagger(\overrightarrow{\mathbf{R}}_i)a(\overrightarrow{\mathbf{R}}_i)+b^\dagger(\overrightarrow{\mathbf{R}}_i)b(\overrightarrow{\mathbf{R}}_i)-a^\dagger(\overrightarrow{\mathbf{R}}_i)b^\dagger(\overrightarrow{\mathbf{R}}_i)-a(\overrightarrow{\mathbf{R}}_i)b(\overrightarrow{\mathbf{R}}_i)\right\rangle \tag{1.114}$$

As before, we can use the translation invariance of $C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)$ to write it as an average over the whole lattice. This allows us to write (1.114) in momentum-space, as follows:

$$C_{AB}(\overrightarrow{\mathbf{k}})\equiv\frac{2}{N}\sum_{\overrightarrow{\mathbf{R}}_i\in\mathscr{L}_{Hex}}C_{AB}(\overrightarrow{\mathbf{k}},\overrightarrow{\mathbf{R}}_i)=\frac{2s}{N}\sum_{\overrightarrow{\mathbf{q}}\in FBZ}\left\langle a^\dagger_{\overrightarrow{\mathbf{q}}}a_{\overrightarrow{\mathbf{q}}}+b^\dagger_{-\overrightarrow{\mathbf{q}}}b_{-\overrightarrow{\mathbf{q}}}-a^\dagger_{\overrightarrow{\mathbf{q}}}b^\dagger_{-\overrightarrow{\mathbf{q}}}-a_{\overrightarrow{\mathbf{q}}}b_{-\overrightarrow{\mathbf{q}}}\right\rangle \tag{1.115}$$

Finally, we must replace the definitions (1.101) into (1.115):

$$C_{AB}(\overrightarrow{\mathbf{k}}) = \frac{2s}{N}\sum_{\overrightarrow{\mathbf{q}}\in FBZ}\Big\langle 2\left\{\cos\phi_{\overrightarrow{\mathbf{q}}}\cosh\eta_{\overrightarrow{\mathbf{q}}}+\sinh\eta_{\overrightarrow{\mathbf{q}}}\right\}\sinh\eta_{\overrightarrow{\mathbf{q}}}+ \\ +\left\{n^c_{\overrightarrow{\mathbf{q}}}+n^d_{\overrightarrow{\mathbf{q}}}\right\}\left(\sinh^2\eta_{\overrightarrow{\mathbf{q}}}+\cosh\eta^2_{\overrightarrow{\mathbf{q}}}-2\cos\phi_{\overrightarrow{\mathbf{q}}}\cosh\eta_{\overrightarrow{\mathbf{q}}}\sinh\eta_{\overrightarrow{\mathbf{q}}}\right)- \\ -c_{\overrightarrow{\mathbf{q}}}d_{\overrightarrow{\mathbf{q}}}\left(e^{i\phi_{\overrightarrow{\mathbf{q}}}}\sinh^2\eta_{\overrightarrow{\mathbf{q}}}+e^{-i\phi_{\overrightarrow{\mathbf{q}}}}\cosh\eta^2_{\overrightarrow{\mathbf{q}}}-2\cosh\eta_{\overrightarrow{\mathbf{q}}}\sinh\eta_{\overrightarrow{\mathbf{q}}}\right)-h.c.\Big\rangle \tag{1.116}$$

From (1.116), we see that, even in the vacuum state, there is a correction to the correlation function, relative to the one expected for the Neél State. Additionally, it is also evident that the correlations between nearest-neighbors (A and B sites) will be exactly the same in both branches. This is vastly different from the results obtained in the FM case.

To finish the calculation of $C_{AB}(\overrightarrow{\mathbf{k}})$, we just replace the $\sinh\eta_{\overrightarrow{\mathbf{q}}}$ and $\cosh\eta_{\overrightarrow{\mathbf{q}}}$ by the values in (1.105), yielding the expression:

$$C_{AB}(\overrightarrow{\mathbf{k}}) = \frac{2s}{N}\sum_{\overrightarrow{\mathbf{q}}\in FBZ}\left[\left\{\frac{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|\cos\phi_{\overrightarrow{\mathbf{q}}}}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|^2}}-1\right\}+\left\{\left\langle n^c_{\overrightarrow{\mathbf{q}}}\right\rangle+\left\langle n^d_{\overrightarrow{\mathbf{q}}}\right\rangle\right\}\left\{\frac{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|\cos\phi_{\overrightarrow{\mathbf{q}}}}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|^2}}\right\}\right. \\ \left.\left\langle c_{\overrightarrow{\mathbf{q}}}d_{\overrightarrow{\mathbf{q}}}\right\rangle\left(\frac{\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|-\cos\phi_{\overrightarrow{\mathbf{q}}}}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|^2}}+i\sin\phi_{\overrightarrow{\mathbf{q}}}\right)+\left\langle c^\dagger_{\overrightarrow{\mathbf{q}}}d^\dagger_{\overrightarrow{\mathbf{q}}}\right\rangle\left(\frac{\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|-\cos\phi_{\overrightarrow{\mathbf{q}}}}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|^2}}-i\sin\phi_{\overrightarrow{\mathbf{q}}}\right)\right] \tag{1.117}$$

For a state containing only one C- or D-type Spin-Wave with momentum $\overrightarrow{\mathbf{k}}$, we get the simplified form:

$$C_{AB}(\overrightarrow{\mathbf{k}}) = -s+\frac{2s}{N}\frac{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|\cos\phi_{\overrightarrow{\mathbf{k}}}}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}+\frac{sv_{cell}}{4\pi^2}\int_{FBZ}d^2\overrightarrow{\mathbf{q}}\,\frac{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|\cos\phi_{\overrightarrow{\mathbf{q}}}}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{q}}}\right|^2}} \tag{1.118}$$

To analyze the expression (1.118), we can start by noticing that $C_{AB}(\overrightarrow{\mathbf{k}}) = \Delta C_0 + F(\overrightarrow{\mathbf{k}})$, where the zero-point contribution — ΔC_0 — was calculated numerically:

$$\Delta C_0 = -0.2099s \tag{1.119}$$

The $\overrightarrow{\mathbf{k}}$-dependent part of (1.118) is seen to diverge in the limit of small-k_y[16]. If the system is at zero temperature, there are no divergences and the only significant feature of the correlation function, is the correction relative to the pure Néel State,:

$$\langle 0|\,\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i)\cdot\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i+\overrightarrow{\delta})\,|0\rangle = -s(s+0.2099) > -s(s+1) \tag{1.120}$$

[16]This is confirmed by an explicit power expansion and it signals that there is no Néel order surviving at finite temperature.

1.4.2.5. Ground-State and Finite Temperature Magnetization

We can now calculate the effect of the Spin-Waves to the order parameter. In this case, that order parameter is the Néel magnetization, as discussed previously:

$$M^z_{Néel} = \left\langle \sum_{i\in\mathscr{L}_{Hex}} \left[S^z(\overrightarrow{\mathbf{R}}_i) - S^z(\overrightarrow{\mathbf{R}}_i + \overrightarrow{\delta}) \right] \right\rangle \tag{1.121}$$

Since the Néel state is not the true ground-state of the system, the spin-wave fluctuations will influence the value of $M_{Néel}$, even in the quantum regime (i.e. $T = 0K$). This effect can be calculated by expressing the operator (1.121), in terms of the normal-mode operators c and d, i.e.:

$$\begin{aligned}\sum_{i\in\mathscr{L}_{Hex}} \left[S^z(\overrightarrow{\mathbf{R}}_i) - S^z(\overrightarrow{\mathbf{R}}_i + \overrightarrow{\delta}) \right] &= Ns \left\{ 1 - \frac{1}{Ns} \sum_{i\in\mathscr{L}_{Hex}} \left[a^\dagger(\overrightarrow{\mathbf{R}}_i) a(\overrightarrow{\mathbf{R}}_i) + b^\dagger(\overrightarrow{\mathbf{R}}_i) b(\overrightarrow{\mathbf{R}}_i) \right] \right\} = \\ &= Ns \left\{ 1 - \frac{1}{Ns} \sum_{\overrightarrow{\mathbf{k}}\in FBZ} \left[a^\dagger_{\overrightarrow{\mathbf{k}}} a_{\overrightarrow{\mathbf{k}}} + b^\dagger_{\overrightarrow{\mathbf{k}}} b_{\overrightarrow{\mathbf{k}}} \right] \right\}\end{aligned} \tag{1.122}$$

Plugging the Bogoliubov-Valatin Transformation in the expression (1.122), we get:

$$\begin{aligned}\sum_{i\in\mathscr{L}_{Hex}} \left[S^z(\overrightarrow{\mathbf{R}}_i) - S^z(\overrightarrow{\mathbf{R}}_i + \overrightarrow{\delta}) \right] = Ns \Bigg\{ 1 - \frac{1}{Ns} \sum_{\overrightarrow{\mathbf{k}}\in FBZ} \Big[2\sinh^2 \eta_{\overrightarrow{\mathbf{k}}} + \left(\cosh^2 \eta_{\overrightarrow{\mathbf{k}}} + \sinh^2 \eta_{\overrightarrow{\mathbf{k}}} \right) \times \\ \times \left(c^\dagger_{\overrightarrow{\mathbf{k}}} c_{\overrightarrow{\mathbf{k}}} + d^\dagger_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} \right) + \sinh 2\eta_{\overrightarrow{\mathbf{k}}} \left(c_{\overrightarrow{\mathbf{k}}} d_{\overrightarrow{\mathbf{k}}} + c^\dagger_{\overrightarrow{\mathbf{k}}} d^\dagger_{\overrightarrow{\mathbf{k}}} \right) \Big] \Bigg\}\end{aligned} \tag{1.123}$$

Now, at $T = 0$ we have the following correction to $M^z_{Néel}$:

$$M^z_{Néel}(T=0) = Ns \left\{ 1 + \frac{1}{2s} - \frac{v_{cell}}{8s\pi^2} \int_{FBZ} d^2\overrightarrow{\mathbf{k}} \frac{1}{\sqrt{1 - \left| \gamma_{\overrightarrow{\mathbf{k}}} \right|^2}} \right\} \tag{1.124}$$

The integral in (1.124) was evaluated numerically, yielding:

$$M^z_{Néel}(T=0) = Ns \left\{ 1 - \frac{1.0164}{s} \right\} \tag{1.125}$$

As expected, the Néel Magnetization is reduced when compared to its value in the Néel State. That reduction is finite in this approximation, which indicates that some degree of long-range order survives in the quantum regime.

At finite temperatures, we must also calculate the contribution to (1.121), coming from the terms proportional to the spin-wave occupation numbers, i.e.:

$$M^z_{N\acute{e}el}(T) = Ns\left\{1 - \frac{1.0164}{s} + \frac{v_{cell}}{8s\pi^2}\int_{FBZ} d^2\overrightarrow{\mathbf{k}}\left\{\frac{\left\langle n^c_{\overrightarrow{\mathbf{k}}}\right\rangle_T + \left\langle n^d_{\overrightarrow{\mathbf{k}}}\right\rangle_T}{\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}\right\}\right\} \tag{1.126}$$

At equilibrium, the occupation numbers for the C- and D-bosons are given by the Planck distribution, meaning that:

$$M^z_{N\acute{e}el}(T) = Ns\left\{1 - \frac{1.0164}{s} + \frac{v_{cell}}{4s\pi^2}\int_{FBZ} d^2\overrightarrow{\mathbf{k}}\left\{\frac{1}{\left(e^{3Js/k_BT\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}-1\right)\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}\right\}\right\} \tag{1.127}$$

Using the fact that $\left|\gamma_{\overrightarrow{\mathbf{k}}}\right| \simeq 1 - \frac{a^2}{12}\left|\overrightarrow{\mathbf{k}}\right|^2 + ...$, we can divide the integral in (1.127) between an integral over a disc D (centered in $\overrightarrow{\mathbf{k}} = 0$ and with radius λ) and its complementary. The integral over the complementary of D is finite, which means that:

$$\int_{FBZ} d^2\overrightarrow{\mathbf{k}}\left\{\frac{1}{\left(e^{3Js/k_BT\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}-1\right)\sqrt{1-\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}}\right\} \simeq$$
$$\simeq (\text{finite part}) + \frac{2\sqrt{6}\pi}{a}\int_0^\lambda dk \frac{k}{\left(e^{(3Ja s/\sqrt{6}k_BT)k+\cdots}-1\right)(k+...)} \to +\infty \tag{1.128}$$

The spin-wave contribution is logarithmically divergent, which is compatible with the result of Mermin-Wagner's Theorem, at finite temperatures.

1.4.3. Interpretation of the Spin-Wave Branches (Equation of Motion Method)

To visualize better the $\overrightarrow{\mathbf{k}} = \overrightarrow{\mathbf{0}}$ spin-waves, we can use the Heisenberg Equation of Motion for the spin operators. Assuming that we will be interested only in states that are invariant under lattice translations, we can suppose that — $\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i)(t) = \overrightarrow{\mathbf{S}}^A(t)$ and $\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_i + \overrightarrow{\delta})(t) = \overrightarrow{\mathbf{S}}^B(t)$, for all $\overrightarrow{\mathbf{R}}_i \in \mathscr{L}_{Hex}$. The equations of motion for the two sublattice operators are:

$$\frac{d\overrightarrow{\mathbf{S}}^A(t)}{dt} = i\left[H, \overrightarrow{\mathbf{S}}^A(t)\right] = 3J\overrightarrow{\mathbf{S}}^A(t)\times\overrightarrow{\mathbf{S}}^B(t) \tag{1.129}$$

$$\frac{d\overrightarrow{\mathbf{S}}^B(t)}{dt} = i\left[H, \overrightarrow{\mathbf{S}}^B(t)\right] = 3J\overrightarrow{\mathbf{S}}^B(t)\times\overrightarrow{\mathbf{S}}^A(t) \tag{1.130}$$

The spin-waves represent small deviations relative to a magnetized state — $\overrightarrow{\mathbf{S}}^A(t) = \overrightarrow{\mathbf{S}}^B(t) = \overrightarrow{\mathbf{M}}$ — which allow us to linearize the equations (1.129) and (1.130) relative to the small fluctuations — $\overrightarrow{\mathbf{h}}^A(t)$ and $\overrightarrow{\mathbf{h}}^B(t)$:

$$\begin{cases} \frac{d\overrightarrow{\mathbf{h}}^A(t)}{dt} &= 3J\overrightarrow{\mathbf{M}} \times \left(\overrightarrow{\mathbf{h}}^B(t) - \overrightarrow{\mathbf{h}}^A(t)\right) \\ \frac{d\overrightarrow{\mathbf{h}}^B(t)}{dt} &= -3J\overrightarrow{\mathbf{M}} \times \left(\overrightarrow{\mathbf{h}}^B(t) - \overrightarrow{\mathbf{h}}^A(t)\right) \end{cases} \Rightarrow \begin{cases} \frac{d}{dt}\left(\overrightarrow{\mathbf{h}}^A(t) + \overrightarrow{\mathbf{h}}^B(t)\right) &= \overrightarrow{\mathbf{0}} \\ \frac{d}{dt}\left(\overrightarrow{\mathbf{h}}^A(t) - \overrightarrow{\mathbf{h}}^B(t)\right) &= -3J\overrightarrow{\mathbf{M}} \times \left(\overrightarrow{\mathbf{h}}^A(t) - \overrightarrow{\mathbf{h}}^B(t)\right) \end{cases} \tag{1.131}$$

This last equations identify clearly the existence of two Γ-pointc modes: One corresponding to a simultaneous rotation of the sublattice magnetizations (which is the Goldstone boson and involves no energy change) and the other corresponding to the existence of opposite spin deviations, in each sublattice, that precess around $\overrightarrow{\mathbf{M}}$ over time. Note that the frequency of precession is $3Js$, as predicted by the dispersion relation calculated in spin-wave theory.

For the AFM case ($J \to -J$), the situation is very similar, the only difference being the fact that the ordered state is — $\overrightarrow{\mathbf{S}}^A(t) = -\overrightarrow{\mathbf{S}}^B(t) = \overrightarrow{\mathbf{M}}$. The final equations of motion for the deviations are:

$$\begin{cases} \frac{d\overrightarrow{\mathbf{h}}^A(t)}{dt} &= 3J\overrightarrow{\mathbf{M}} \times \left(\overrightarrow{\mathbf{h}}^B(t) + \overrightarrow{\mathbf{h}}^A(t)\right) \\ \frac{d\overrightarrow{\mathbf{h}}^B(t)}{dt} &= -3J\overrightarrow{\mathbf{M}} \times \left(\overrightarrow{\mathbf{h}}^B(t) + \overrightarrow{\mathbf{h}}^A(t)\right) \end{cases} \Rightarrow \begin{cases} \frac{d}{dt}\left(\overrightarrow{\mathbf{h}}^A(t) + \overrightarrow{\mathbf{h}}^B(t)\right) &= \overrightarrow{\mathbf{0}} \\ \frac{d}{dt}\left(\overrightarrow{\mathbf{h}}^A(t) - \overrightarrow{\mathbf{h}}^B(t)\right) &= -3J\overrightarrow{\mathbf{M}} \times \left(\overrightarrow{\mathbf{h}}^A(t) + \overrightarrow{\mathbf{h}}^B(t)\right) \end{cases} \tag{1.132}$$

The interpretation of the first mode in (1.132) seems to be similar to the ferromagnetic case — a global rotation of all the spins. The second case is more difficult to interpret, since it seems to diverge in time, which signals an instability of the Neél state. As far as we can see, this is related with the fact that, even at this level of approximation, the ground-state is not a Néel state, but a quantum condensate of spin-waves.

1.4.4. The Easy-Axis Anisotropic AFM in the Graphene Lattice

Up until now, we have been exploring the isotropic Heisenberg model. In all the cases, because the system is two-dimensional, we have seen that no long-range magnetic order seems to survive thermal fluctuations. However, following the suggestion made by P. W. Anderson [2], we can avoid all the divergences in the calculations by adding an anisotropic term in the Hamiltonian, which breaks the rotational symmetry[17]. In fact, this anisotropy can be as small as we wish, and order will still prevail at finite temperatures.

In this last subsection, we will explore this possibility, using Spin-Wave theory.

1.4.4.1. Building the Hamiltonian

We start by the following AFM Hamiltonian:

[17] Next chapter, we will see that the Mermin-Wagner Theorem is only valid for isotropic models.

$$H = J \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \left\{ \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i + \vec{\delta}) + \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1 + \vec{\delta}) + \vec{\mathbf{S}}(\vec{\mathbf{R}}_i) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2 + \vec{\delta}) \right\}$$
$$- \frac{J\alpha}{2} \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \left\{ \left(S^z(\vec{\mathbf{R}}_i) \right)^2 + \left(S^z(\vec{\mathbf{R}}_i + \vec{\delta}) \right)^2 \right\}; \quad \text{with } J > 0 \text{ and } \alpha \ll 1 \tag{1.133}$$

The $O(3)$ symmetry is explicitly broken and reduced to the set of arbitrary rotations around the $\hat{z}$-axis ($O(2)$-symmetry). Hence the $\hat{z}$-direction is the preferred direction here.

From now on, we will apply exactly the same procedure to the new Hamiltonian (1.133), starting by expressing it in terms of HP operators:

$$H_A = -\frac{3Js^2N}{2}\left(1 + \frac{\alpha}{3}\right) + Js \sum_{\vec{\mathbf{R}}_i \in \mathscr{L}_{Hex}} \Big[(1+\alpha)\, b^\dagger(\vec{\mathbf{R}}_i) b(\vec{\mathbf{R}}_i) + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) +$$
$$+ b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) + (3+\alpha)\, a^\dagger(\vec{\mathbf{R}}_i) a(\vec{\mathbf{R}}_i) - a^\dagger(\vec{\mathbf{R}}_i) \Big\{ b^\dagger(\vec{\mathbf{R}}_i) +$$
$$+ b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + b^\dagger(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) \Big\} - a(\vec{\mathbf{R}}_i) \Big\{ b(\vec{\mathbf{R}}_i) + b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_1) + b(\vec{\mathbf{R}}_i - \vec{\mathbf{a}}_2) \Big\} + \mathcal{O}(1/s) \Big] \tag{1.134}$$

In momentum-space, one gets:

$$H_A = -\frac{3Js^2N}{2}\left(1 + \frac{\alpha}{3}\right) + (3+\alpha)\, Js \sum_{\vec{\mathbf{k}} \in FBZ} \left[b^\dagger_{-\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}} + a^\dagger_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} - \beta^*_{\vec{\mathbf{k}}} a^\dagger_{\vec{\mathbf{k}}} b^\dagger_{-\vec{\mathbf{k}}} - \beta_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}} b_{-\vec{\mathbf{k}}} \right] \tag{1.135}$$

Where the new parameter is — $\beta_{\vec{\mathbf{k}}} = \frac{3}{3+\alpha}\gamma_{\vec{\mathbf{k}}} = \frac{1}{3-\alpha}\left\{1 + e^{i\vec{\mathbf{a}}_1 \cdot \vec{\mathbf{k}}} + e^{i\vec{\mathbf{a}}_2 \cdot \vec{\mathbf{k}}}\right\}$.

1.4.4.2. Diagonalizing the Hamiltonian

To diagonalize (1.135), we must find a new Bogoliubov-Valatin Transformation that will eliminate the non-conserving terms. However, since we can obtain (1.135) from (1.106) just by replacing $J \to J(1 + \alpha/3)$ and $\gamma_{\vec{\mathbf{k}}} \to \beta_{\vec{\mathbf{k}}}$, we can guess the form of the transformation by inspection:

$$\begin{cases} a_{\vec{\mathbf{k}}} = \cosh\eta_{\vec{\mathbf{k}}} c_{\vec{\mathbf{k}}} + \sinh\eta_{\vec{\mathbf{k}}} d^\dagger_{\vec{\mathbf{k}}} \\ a^\dagger_{\vec{\mathbf{k}}} = \cosh\eta_{\vec{\mathbf{k}}} c^\dagger_{\vec{\mathbf{k}}} + \sinh\eta_{\vec{\mathbf{k}}} d_{\vec{\mathbf{k}}} \end{cases} \qquad \begin{cases} b_{-\vec{\mathbf{k}}} = e^{-i\phi_{\vec{\mathbf{k}}}} \cosh\eta_{\mathbf{k}} d_{\mathbf{k}} + e^{-i\phi_{\vec{\mathbf{k}}}} \sinh\eta_{\mathbf{k}} c^\dagger_{\mathbf{k}} \\ b^\dagger_{-\vec{\mathbf{k}}} = e^{i\phi_{\vec{\mathbf{k}}}} \cosh\eta_{\mathbf{k}} d^\dagger_{\mathbf{k}} + e^{i\phi_{\vec{\mathbf{k}}}} \sinh\eta_{\mathbf{k}} c_{\mathbf{k}} \end{cases} \tag{1.136}$$

With the parameters:

$$\begin{aligned} \cosh\eta_{\vec{\mathbf{k}}} &= \sqrt{\frac{1}{2}\sqrt{\frac{1}{1 - \frac{1}{(1+\alpha/3)^2}|\gamma_{\vec{\mathbf{k}}}|^2}} + \frac{1}{2}} \\ \sinh\eta_{\vec{\mathbf{k}}} &= \sqrt{\frac{1}{2}\sqrt{\frac{1}{1 - \frac{1}{(1+\alpha/3)^2}|\gamma_{\vec{\mathbf{k}}}|^2}} - \frac{1}{2}} \end{aligned} \tag{1.137}$$

By doing the proper replacement in (1.135), we get the following diagonal form:

$$H_A = -\frac{3J(1+\alpha/3)s(s+1)N}{2} + 3J(1+\alpha/3)s \sum_{\vec{\mathbf{k}}\in FBZ} \left[\left\{ \sqrt{1 - \frac{1}{(1+\alpha/3)^2} \left|\gamma_{\vec{\mathbf{k}}}\right|^2} \right\} \times \right.$$
$$\left. \times \left(c^\dagger_{\vec{\mathbf{k}}} c_{\vec{\mathbf{k}}} + d^\dagger_{\vec{\mathbf{k}}} d_{\vec{\mathbf{k}}} \right) \right] + 3J(1+\alpha/3)s \sum_{\vec{\mathbf{k}}\in FBZ} \sqrt{1 - \frac{1}{(1+\alpha/3)^2} \left|\gamma_{\vec{\mathbf{k}}}\right|^2} \tag{1.138}$$

The dispersion relation for the spin-waves, as well as the energy of the ground-state, are now altered by the parameter α. The long-wavelength expansion for the new spectrum goes as follows:

$$\epsilon(\vec{\mathbf{k}}) = 3Js\,(1+\alpha/3) \sqrt{\left(1 - \frac{1}{(1+\alpha/3)^2}\right) + \frac{a^2}{12\,(1+\alpha/3)^2} \left|\vec{\mathbf{k}}\right|^2 + \ldots} \sim$$
$$\sim Js\sqrt{6}\sqrt{(1+\alpha/3)^2 - 1} \left\{ 1 + \frac{a^2}{12\left[(1+\alpha/3)^2 - 1\right]} \left|\vec{\mathbf{k}}\right|^2 + \ldots \right\} \tag{1.139}$$

According to (1.139), the presence of the anisotropic term generates a gap in the Spin-Wave Spectrum — $\Delta_g = Js\sqrt{6}\sqrt{(1+\alpha/3)^2 - 1}$ — and a quadratic dispersion relation for the long-wavelength modes. This can be seen in the 3-D plot of Figure 1.5 and is in sharp contrast with the result obtained for the isotropic case.

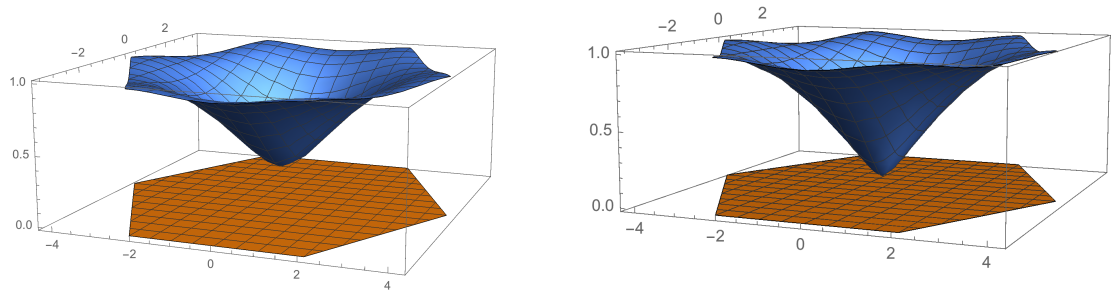


Figure 1.5.: 3D Plots of the Spin-Wave Dispersion Relation for both branches obtained in the anisotropic AFM case. The values used for the anisotropy parameter were $\alpha = 0.1$(on the left) and $\alpha = 0.01$ (on the right).

To see what is the effect of this anisotropy in the physical properties of the system, we can recalculate the Néel magnetization at finite temperature. So, we take the expression (1.128), and make the required modifications:

$$\int_{FBZ} d^2\overrightarrow{\mathbf{k}} \left\{ \frac{1}{\left(e^{3J(1+\alpha/3)s/k_BT\sqrt{1-\frac{1}{(1+\alpha/3)^2}\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}} - 1 \right)\sqrt{1-\frac{1}{(1+\alpha/3)^2}\left|\gamma_{\overrightarrow{\mathbf{k}}}\right|^2}} \right\} \simeq$$

$$\simeq Finite + \frac{2\sqrt{6}\pi}{a}\int_0^\lambda dk \frac{k}{\left(e^{\frac{\Delta_g}{k_BT}+\frac{P}{k_BT}k^2+\ldots} - 1 \right)(\Delta_g + Pk^2 + ...)} \tag{1.140}$$

Where $P = \frac{Js\sqrt{6}}{\sqrt{(1+\alpha/3)^2-1}}$.

As long as α and $P\left|\overrightarrow{\mathbf{k}}\right|^2$ are small when compared with k_BT, we can expand the exponential in powers of its argument. This yields:

$$\int_0^\lambda dk \frac{k}{\left(e^{\frac{\Delta_g}{k_BT}+\frac{P}{k_BT}k^2+\ldots} - 1 \right)(\Delta_g + Pk^2 + ...)} \simeq k_BT \times \int_0^\lambda dk \frac{k}{(\Delta_g + Pk^2 + ...)^2} \tag{1.141}$$

This integral is convergent. So, as expected, the anisotropic term (no matter how small it is) will always stabilize the long-ranged AFM order, with respect to thermal fluctuations. It acts as a regulator for the integrals over $\overrightarrow{\mathbf{k}}$.

1.5. The Failure of Spin-Wave Theory at Low-Dimensions (A Reflection)

In this chapter, we have taken a first approach to understanding the microscopic physics behind magnetism, by studying lattices of quantum spins interacting via the Heisenberg Hamiltonian. In essence, we have guessed a ground-state configuration for the system, and expanded the spin Hamiltonian in terms of bosonic excitations that were non-interacting in first-order. By diagonalizing this effective Hamiltonian, we have been able to obtain approximate dispersion relations for this low-energy modes, in both the ferro- and anti-ferromagnetic models.

For both cases, we have used these results to predict physical observables, and obtained divergences in at any finite temperatures, for the one- and two-dimensional systems.

Furthermore, in the AFM chain, we have even obtained diverging corrections to the magnetization at $T = 0$, which seems to be an indication that maybe even the ground-state of this system is magnetically disordered. This conclusion is known to be true exactly for the spin-1/2 chain, as referred in [6].

All these ill-behaved results are difficult to interpret, as they are. In fact, they can be seen as signs that our approximate scheme does not work for those cases, and new routes must be taken to deal with them. Therefore, we will take this failure as our starting point for motivating all the upcoming discussion, where we will employ deeper theoretical tools to explain this failure and, hopefully, be able to make actual predictions for low-dimensional systems.

[This page was intentionally left blank]

2. Magnetic Order and Exact Results in the Heisenberg Model

In the last chapter, we have explored some simple and reasonable models for a lattice of interacting spins. The main reason for doing it was to see if such microscopic models were capable of producing physical predictions compatible with the existence of spontaneous magnetization and antiferromagnetism (both of these phenomena are established experimentally). Both forms of magnetic order are just special cases of spontaneous symmetry-breaking, a central concept in several physical theories.

In this chapter, we intend to clarify the physical (and mathematical) meaning of spontaneous symmetry-breaking and prove a rigorous theorem regarding long-range order in low-dimensional systems (the Mermin-Wagner Theorem) that will shine some light on the interpretation of the results of last chapter. In the second part, we will prove some rigorous results regarding the true ground-state of the unfrustrated Heisenberg antiferromagnetic model, that will serve as a theoretical basis for our following study of quantum spin systems.

2.1. What Is A Magnetically Ordered Phase?

In what follows, we will take the general the isotropic Heisenberg Model placed on a Bravais Lattice, as our model Hamiltonian. This is given, again by (2.1):

$$H_{Heis} = \sum_{\vec{\mathbf{R}}_1 \in \mathscr{L}} \sum_{\vec{\mathbf{R}}_2 \in \mathscr{L}} J\left(\vec{\mathbf{R}}_2 - \vec{\mathbf{R}}_1\right) \vec{\mathbf{S}}(\vec{\mathbf{R}}_1) \cdot \vec{\mathbf{S}}(\vec{\mathbf{R}}_2) - B \sum_{\vec{\mathbf{R}}_1 \in \mathscr{L}} S^z(\vec{\mathbf{R}}_1) e^{-i\vec{\mathbf{Q}}\cdot\vec{\mathbf{R}}_1} \tag{2.1}$$

Here, $J\left(\vec{\mathbf{R}}_2 - \vec{\mathbf{R}}_1\right)$ is the spin-spin coupling function and B represents the magnitude of an external space-dependent magnetic field (multiplied by the gyromagnetic ratio appropriate to the system in question).

This model, in case $B = 0$, is invariant under space-rotations around any axis and lattice translations. This means that all the eigenstates of (2.1) can be collected into representations of the associated groups. In particular, the system will not distinguish among states that are magnetized in different directions of space.

The interesting question is to see if it is possible at $T = 0K$ (quantum regime) or $T > 0K$, for the system to be in a stable state which favors a given direction in space — i.e. where the rotation symmetry lies broken. This is the essence of the symmetry-breaking phenomenon that we wish to define.

As a first trial, we can define a symmetry-broken state (quantum or thermal) as one in which the value of the magnetization remains finite even when one takes the external field to zero $B \to 0$. We define (2.2) as the non-uniform magnetization operator:[1]

$$M^z(\overrightarrow{\mathbf{Q}}) = \frac{1}{N v_{cell}} \sum_{\overrightarrow{\mathbf{R}}_1 \in \mathscr{L}} S^z(\overrightarrow{\mathbf{R}}_1) e^{-i\overrightarrow{\mathbf{Q}}\cdot\overrightarrow{\mathbf{R}}_1} \tag{2.2}$$

Then, we say that the system is in a symmetry-broken state if the following holds (for a temperature T and an external field $\mathbf{B}$):

$$\left| \lim_{B\to 0} \left\langle M^z(\overrightarrow{\mathbf{Q}}) \right\rangle_{T,B,N} \right| \geq 0 \tag{2.3}$$

Despite the reasonability of the above definition, one must think in which cases can it be satisfied. And the truth is that (2.3) is not verified by any finite lattice model, at a finite temperature. This can be inferred from the following argumentation:

1. By symmetry, any given energy eigenstate $|\psi_+\rangle$ with magnetization $\langle\psi_+| M^z(\overrightarrow{\mathbf{Q}}) |\psi_+\rangle = C > 0$, has a counterpart eigenvector — $|\psi_-\rangle$ — with the same energy, but rotated 180^{o} relative to the y-axis (i.e. with $\langle\psi_-| M^z(\overrightarrow{\mathbf{Q}}) |\psi_-\rangle = -C$).
2. At finite temperatures, both of these states have an occupation probability equal to $e^{-\beta E}$, meaning that the overall average value of the magnetization will be null in any canonical thermal state.

At zero temperature, on the other hand, one can have the system at a stationary state that has a non-zero magnetization[2]. But even then, there are many important cases in which the order parameter does not commute with (2.1), which means that a magnetized state will not be stable under time evolution.

Therefore, one sees that the definition (2.3) is too restrictive to be of any use in real systems. Building on the ideas of P. W. Anderson [2,5], we must change (2.3) by going to the thermodynamic limit (or better, a thermodynamic limit) before taking $B \to 0$, as follows:

$$\left| \lim_{B\to 0} \left[\lim_{N\to\infty} \left[\left\langle M^z(\overrightarrow{\mathbf{Q}}) \right\rangle_{T,B,N} \right] \right] \right| \geq 0 \tag{2.4}$$

Usually, a broken state — (2.4) — is also called a magnetically ordered state. The reason for that is the fact that such a state will always exhibit a spin-spin correlation function which decays (with distance) to a finite value instead of decaying to zero. This is what we call long-range order (LRO). Defining the spin-spin correlation function as in (2.5), we can prove that (2.4) implies the existence of LRO in the system:

$$C_{T,B,N}(\overrightarrow{\delta}) = \frac{1}{N} \sum_{\overrightarrow{\mathbf{R}}\in\mathscr{L}} \left\langle \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}) \cdot \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}} + \overrightarrow{\delta}) \right\rangle_{T,B,N} \tag{2.5}$$

[1] Notice that this choice of order parameter contemplates both the ferromagnetic — $\overrightarrow{\mathbf{Q}} = \overrightarrow{\mathbf{0}}$ — and also antiferromagnetic, if we choose $\overrightarrow{\mathbf{Q}}$ to satisfy $\overrightarrow{\mathbf{Q}} \cdot \overrightarrow{\mathbf{R}} = \pi n$, with $n \in \mathbb{N}$, for all $\overrightarrow{\mathbf{R}}$ being a vector that connects two different sublattices.

[2] This happens provided that the magnetization is a good quantum number of system. This was the case of the Heisenberg FM model studied in the last chapter.

One can take its Fourier Transform easily, by using the definition $\overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{q}}} = \frac{1}{N}\sum_j \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_j)e^{i\overrightarrow{\mathbf{q}}\cdot\overrightarrow{\mathbf{R}}_j}$, yielding:

$$C_{T,B,N}(\overrightarrow{\delta}) = \sum_{\overrightarrow{\mathbf{q}}\in FBZ} \left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{q}}} \cdot \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{q}}} \right\rangle_{T,B,N} e^{i\overrightarrow{\delta}\cdot\overrightarrow{\mathbf{q}}} \tag{2.6}$$

Now, we can prove the inequality (2.7) by using the Cauchy-Schwartz inequality for the internal product of vectors.

$$0 \leq \left|\left\langle \overrightarrow{\mathbf{M}}(\overrightarrow{\mathbf{Q}})\right\rangle\right|^2 \leq \left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{Q}}} \cdot \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N} \tag{2.7}$$

The proof goes as follows:

$$\begin{aligned}\left|\left\langle \overrightarrow{\mathbf{M}}(\overrightarrow{\mathbf{Q}})\right\rangle\right|^2 = \left\langle \overrightarrow{\mathbf{M}}(\overrightarrow{\mathbf{Q}})\right\rangle \cdot \left\langle \overrightarrow{\mathbf{M}}(-\overrightarrow{\mathbf{Q}})\right\rangle \leq \left|\left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{Q}}}\right\rangle_{T,B,N}\right| \left|\left\langle \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{Q}}}\right\rangle_{T,B,N}\right| \leq \\ \leq \left\langle \left|\overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{Q}}}\right|^2 \right\rangle_{T,B,N} = \left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{Q}}} \cdot \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N}\end{aligned}$$

In the absence of order, the spin correlations are short-ranged[3] and insensitive to the increase in the number of spins. This means the following:

$$\left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{q}}} \cdot \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{q}}} \right\rangle = \frac{1}{N}\sum_{\overrightarrow{\mathbf{R}}\in\mathscr{L}} \left\langle \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{0}}) \cdot \overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}) \right\rangle e^{i\overrightarrow{\mathbf{q}}\cdot\overrightarrow{\mathbf{R}}} \sim \mathcal{O}\left(\frac{1}{N}\right) \tag{2.8}$$

However, because of the result (2.7), we know that for the particular $\overrightarrow{\mathbf{Q}}$ related to the order parameter, we must have:

$$0 < \lim_{B\to 0}\left[\lim_{N\to 0}\left|\left\langle \overrightarrow{\mathbf{M}}(\overrightarrow{\mathbf{Q}})\right\rangle\right|^2\right] \leq \lim_{B\to 0}\left[\lim_{N\to 0}\left[\left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{Q}}} \cdot \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N}\right]\right] \tag{2.9}$$

And this inequality guarantees that, for a magnetized system:

$$\left\langle \overrightarrow{\mathbf{S}}_{\overrightarrow{\mathbf{Q}}} \cdot \overrightarrow{\mathbf{S}}_{-\overrightarrow{\mathbf{Q}}} \right\rangle \sim \mathcal{O}(1)$$

Which is in contradiction with the result (2.8), meaning that that the spin correlation function must not be short-ranged for this case. The asymptotic behavior of the correlations will be of the form:.

$$C_{T,B=0,\infty}(\overrightarrow{\delta}) \to (\text{constant}) \times \cos\left(\overrightarrow{\delta}\cdot\overrightarrow{\mathbf{Q}}\right)$$

2.2. The Mermin-Wagner Theorem

References: [4,7]

[3] If we assume a local Hamiltonian, this is certainly true.

In this section, we will try to prove, that it is not possible to a have spontaneous magnetization on any isotropic Heisenberg Model, as long as the couplings are short-ranged and the lattice is one- or two-dimensional. This is the content of the so called **Mermin-Wagner Theorem** (MWT).

The proof we will follow here is based on the original reference [4], and makes use of the Bogoliubov inequality, which we state as follows (and prove in the [Appendix B.1]):

Bogoliubov Inequality:

Let A and C be two operators acting on the Hilbert Space $\mathscr{H}$, spanned by a set of eigenvectors of an arbitrary Hamiltonian H. Then, at a finite temperature T, the following inequality is true:

$$\left\langle \left\{ A, A^\dagger \right\} \right\rangle_T \left\langle \left[C^\dagger, [H, C] \right] \right\rangle_T \geq 2k_B T \left| \left\langle \left[C^\dagger, A^\dagger \right] \right\rangle_T \right|^2 \tag{2.10}$$

All the averages are taken in a canonical thermal state —$\langle ... \rangle_T = {}^1/_Z Tr\left\{ e^{-\beta H} ... \right\}$.

2.2.1. The Mermin-Wagner Bound in the Heisenberg Model

Despite of its sterile look, the inequality (2.10) can be used in the derivation of some exact results, concerning symmetry-breaking in low-dimensional systems, at finite temperatures. In particular, it allows the establishment of **a precise bound in the magnetization for the Heisenberg model,** that rules out any possibility of long-range order for 1- and 2-dimensional lattices. To obtain that, that we must start by defining the Lattice Fourier Transform of the spin operators (and its inverse):

$$S^\alpha_{\vec{\mathbf{k}}} = \frac{1}{N} \sum_{\vec{\mathbf{R}} \in \mathscr{L}} S^\alpha(\vec{\mathbf{R}}) e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}} \tag{2.11}$$

$$S^\alpha(\vec{\mathbf{R}}) = \sum_{\vec{\mathbf{k}} \in FBZ} S^\alpha_{\vec{\mathbf{k}}} e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}} \tag{2.12}$$

This allow us to write the following commutation relations:

$$\begin{aligned} \left[S^\pm_{\vec{\mathbf{k}}}, S^z_{\vec{\mathbf{q}}} \right] &= \frac{1}{N^2} \sum_{\vec{\mathbf{R}}_1, \vec{\mathbf{R}}_2} \left[S^\pm(\vec{\mathbf{R}}_1), S^z(\vec{\mathbf{R}}_2) \right] e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_1 + i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}_2} = \\ &= \mp \frac{1}{N^2} \sum_{\vec{\mathbf{R}}_1, \vec{\mathbf{R}}_2} S^\pm(\vec{\mathbf{R}}_1) \delta_{\vec{\mathbf{R}}_1, \vec{\mathbf{R}}_2} e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_1 + i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}_2} = \mp \frac{1}{N} S^\pm_{\vec{\mathbf{k}}+\vec{\mathbf{q}}} \end{aligned} \tag{2.13}$$

$$\left[S^+_{\vec{\mathbf{k}}}, S^-_{\vec{\mathbf{q}}}\right] = \frac{1}{N^2}\sum_{\vec{\mathbf{R}}_1,\vec{\mathbf{R}}_2}\left[S^+(\vec{\mathbf{R}}_1), S^-(\vec{\mathbf{R}}_2)\right]e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_1+i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}_2} =$$
$$= \frac{2}{N^2}\sum_{\vec{\mathbf{R}}_1,\vec{\mathbf{R}}_2} S^z(\vec{\mathbf{R}}_1)\delta_{\vec{\mathbf{R}}_1,\vec{\mathbf{R}}_2}e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_1+i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}_2} = \frac{2}{N}S^z_{\vec{\mathbf{k}}+\vec{\mathbf{q}}} \tag{2.14}$$

We can also rewrite the Hamiltonian (2.1), in terms of these momentum-space operators, yielding[4]:

$$H_{Heis} = \sum_{\vec{\mathbf{k}},\vec{\mathbf{p}},\vec{\mathbf{q}}} J_{\vec{\mathbf{k}}}\,\vec{\mathbf{S}}_{\vec{\mathbf{q}}}\cdot\vec{\mathbf{S}}_{\vec{\mathbf{p}}}\sum_{\vec{\mathbf{R}}_1,\vec{\mathbf{R}}_2} e^{-i\vec{\mathbf{k}}\cdot(\vec{\mathbf{R}}_2-\vec{\mathbf{R}}_1)}e^{-i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}_1}e^{-i\vec{\mathbf{p}}\cdot\vec{\mathbf{R}}_2} - NBS^z_{\vec{\mathbf{Q}}} =$$
$$= \sum_{\vec{\mathbf{k}},\vec{\mathbf{p}},\vec{\mathbf{q}}} J_{\vec{\mathbf{k}}}\,\vec{\mathbf{S}}_{\vec{\mathbf{q}}}\cdot\vec{\mathbf{S}}_{\vec{\mathbf{p}}}\sum_{\vec{\mathbf{R}}_1,\vec{\mathbf{R}}_2} e^{-i(\vec{\mathbf{p}}-\vec{\mathbf{k}})\cdot\vec{\mathbf{R}}_1}e^{-i(\vec{\mathbf{q}}+\vec{\mathbf{p}})\cdot\vec{\mathbf{R}}_2} - NBS^z_{\vec{\mathbf{Q}}} =$$
$$= N^2\sum_{\vec{\mathbf{k}}\in FBZ} J_{\vec{\mathbf{k}}}\,\vec{\mathbf{S}}_{\vec{\mathbf{k}}}\cdot\vec{\mathbf{S}}_{-\vec{\mathbf{k}}} - NBS^z_{\vec{\mathbf{Q}}} \tag{2.15}$$

Now, we can follow the method devised in [4] and choose the following operators — $C = S^+_{\vec{\mathbf{p}}}$ and $A = S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}$. Then, we need to calculate the double-commutator defined as:

$$D_{\vec{\mathbf{p}}}(\vec{\mathbf{Q}}) \equiv \left\langle\left[S^-_{-\vec{\mathbf{p}}}, \left[H\left(\vec{\mathbf{Q}}\right), S^+_{\vec{\mathbf{p}}}\right]\right]\right\rangle_{T,B,N} \tag{2.16}$$

This is done as follows:

$$\left[H, S^+_{\vec{\mathbf{p}}}\right] = N^2\sum_{\vec{\mathbf{k}}\in FBZ} J_{\vec{\mathbf{k}}}\left[S^z_{\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{k}}} + 1/2\left(S^-_{\vec{\mathbf{k}}}S^+_{-\vec{\mathbf{k}}}, +S^+_{\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{k}}}\right), S^+_{\vec{\mathbf{p}}}\right] - NB\left[S^z_{\vec{\mathbf{Q}}}, S^+_{\vec{\mathbf{p}}}\right] =$$
$$= N\sum_{\vec{\mathbf{k}}\in FBZ} J_{\vec{\mathbf{k}}}\left[S^z_{\vec{\mathbf{k}}}S^+_{\vec{\mathbf{p}}-\vec{\mathbf{k}}} + S^+_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{k}}} - S^z_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}S^+_{-\vec{\mathbf{k}}} - S^+_{\vec{\mathbf{k}}}S^z_{\vec{\mathbf{p}}-\vec{\mathbf{k}}}\right] - BS^+_{\vec{\mathbf{Q}}+\vec{\mathbf{p}}} = \tag{2.17}$$

$$\left[S^-_{-\vec{\mathbf{p}}}, \left[H, S^+_{\vec{\mathbf{p}}}\right]\right] = \sum_{\vec{\mathbf{k}}\in FBZ} J_{\vec{\mathbf{k}}}\left[S^-_{\vec{\mathbf{k}}-\vec{\mathbf{p}}}S^+_{\vec{\mathbf{p}}-\vec{\mathbf{k}}} - 4S^z_{\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{k}}} + S^+_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{k}}} -\right.$$
$$\left. - S^-_{\vec{\mathbf{k}}}S^+_{-\vec{\mathbf{k}}} + 2S^z_{\vec{\mathbf{p}}+\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{p}}-\vec{\mathbf{k}}} + 2S^z_{\vec{\mathbf{k}}-\vec{\mathbf{p}}}S^z_{\vec{\mathbf{p}}-\vec{\mathbf{k}}} - S^+_{\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{k}}}\right] + \frac{2B}{N}S^z_{\vec{\mathbf{Q}}} \tag{2.18}$$

The last sum can be re-organized by shifting the summed momentum vectors and using the property — $J_{-\vec{\mathbf{k}}} = J_{\vec{\mathbf{k}}}$ — yielding:

[4]Notice that the function $J(\vec{\mathbf{R}})$ is also a real-valued function defined on the lattice and an even function — $J(-\vec{\mathbf{R}}) = J(\vec{\mathbf{R}})$.

$$\begin{aligned}\left[S^-_{-\vec{\mathbf{p}}},\left[H,S^+_{\vec{\mathbf{p}}}\right]\right] &= \sum_{\vec{\mathbf{k}}\in FBZ} J_{\vec{\mathbf{k}}}\left[S^-_{\vec{\mathbf{k}}-\vec{\mathbf{p}}}S^+_{\vec{\mathbf{p}}-\vec{\mathbf{k}}} - 4S^z_{\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{k}}} + S^+_{\vec{\mathbf{p}}-\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{p}}+\vec{\mathbf{k}}} - \right.\\ &\left. - S^-_{\vec{\mathbf{k}}}S^+_{-\vec{\mathbf{k}}} + 2S^z_{\vec{\mathbf{p}}-\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{p}}+\vec{\mathbf{k}}} + 2S^z_{\vec{\mathbf{k}}-\vec{\mathbf{p}}}S^z_{\vec{\mathbf{p}}-\vec{\mathbf{k}}} - S^+_{\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{k}}}\right] + \frac{2B}{N}S^z_{\vec{\mathbf{Q}}} =\\ &= -\sum_{\vec{\mathbf{k}}\in FBZ}\left[J_{\vec{\mathbf{k}}} - J_{\vec{\mathbf{k}}+\vec{\mathbf{p}}}\right]\left[S^-_{\vec{\mathbf{k}}}S^+_{-\vec{\mathbf{k}}} + S^+_{\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{k}}} + 4S^z_{\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{k}}}\right] + \frac{2B}{N}S^z_{\vec{\mathbf{Q}}} \end{aligned} \tag{2.19}$$

At last, we can write the final expression for $D_{\vec{\mathbf{p}}}(\vec{\mathbf{Q}})$, i.e.:

$$D_{\vec{\mathbf{p}}}(\vec{\mathbf{Q}}) = -\sum_{\vec{\mathbf{k}}\in FBZ}\left[J_{\vec{\mathbf{k}}} - J_{\vec{\mathbf{k}}+\vec{\mathbf{p}}}\right]\left\langle S^-_{\vec{\mathbf{k}}}S^+_{-\vec{\mathbf{k}}} + S^+_{\vec{\mathbf{k}}}S^-_{-\vec{\mathbf{k}}} + 4S^z_{\vec{\mathbf{k}}}S^z_{-\vec{\mathbf{k}}}\right\rangle_{T,B,N} + \frac{2Bv_{cell}}{N}\left\langle m^z_{\vec{\mathbf{Q}}}\right\rangle_{T,B,N} \tag{2.20}$$

Where we have identified the last term as being the $\vec{\mathbf{Q}}$-th Fourier component of the magnetization density along the z-axis. In the same way, we need to calculate the two other terms that will enter in the Bogoliubov Inequality, i.e.:

$$\left\langle\left[C^\dagger, A^\dagger\right]\right\rangle_{T,B,N} = \left\langle\left[S^-_{-\vec{\mathbf{p}}}, S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}}\right]\right\rangle_{T,B,N} = -\frac{2v_{cell}}{N}\left\langle m^z_{\vec{\mathbf{Q}}}\right\rangle_{T,B,N} \tag{2.21}$$

$$\left\langle\left\{A, A^\dagger\right\}\right\rangle_{T,B,N} = \left\langle S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}} + S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}}S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}\right\rangle_{T,B,N} \tag{2.22}$$

Plugging (2.20)-(2.22) in the inequality (2.10), we get:

$$\left\langle S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}} + S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}}S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}\right\rangle_{T,B,N} \geq \frac{8k_BTv^2_{cell}}{N^2 D_{\vec{\mathbf{p}}}(\vec{\mathbf{Q}})}\left\langle m^z_{\vec{\mathbf{Q}}}\right\rangle^2_{T,B,N} \tag{2.23}$$

Obviously, one can sum both sides over the whole FBZ of the lattice, and still maintain the inequality. By doing this, we can obtain the following bound for the left-hand side of (2.23):

$$\begin{aligned}&\sum_{\vec{\mathbf{p}}}\left\langle S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}} + S^+_{\vec{\mathbf{p}}+\vec{\mathbf{Q}}}S^-_{-\vec{\mathbf{p}}-\vec{\mathbf{Q}}}\right\rangle_{T,B,N} =\\ &= \frac{1}{N^2}\sum_{\vec{\mathbf{p}}}\sum_{\vec{\mathbf{R}}_1\vec{\mathbf{R}}_2}\left\langle S^+(\vec{\mathbf{R}}_1)S^-(\vec{\mathbf{R}}_2) + S^-(\vec{\mathbf{R}}_2)S^+(\vec{\mathbf{R}}_1)\right\rangle e^{-i\left(\vec{\mathbf{p}}+\vec{\mathbf{Q}}\right)\cdot\left(\vec{\mathbf{R}}_1-\vec{\mathbf{R}}_2\right)} =\\ &= \frac{2}{N}\sum_{\vec{\mathbf{R}}}\left\langle S^2(\vec{\mathbf{R}}) - S^z(\vec{\mathbf{R}})S^z(\vec{\mathbf{R}})\right\rangle \leq 2S(S+1)\end{aligned} \tag{2.24}$$

Which allows us to write the following:

$$S(S+1) \geq 4k_BTv^2_{cell}\left\langle m^z_{\vec{\mathbf{Q}}}\right\rangle^2_{T,B,N}\left[\frac{1}{N^2}\sum_{\vec{\mathbf{p}}\in FBZ}\frac{1}{D_{\vec{\mathbf{p}}}(\vec{\mathbf{Q}})}\right] \tag{2.25}$$

The only thing that remains to be done is to find a suitable bound for the double commutator $D_{\overrightarrow{\mathbf{p}}}(\overrightarrow{\mathbf{Q}})$. First of all, it is clear that $D_{\overrightarrow{\mathbf{p}}}(\overrightarrow{\mathbf{Q}}) \geq 0$, since it represents the squared-norm of the operator $B = \left[S^-_{-\overrightarrow{\mathbf{p}}}, H\right]$. Hence, we can say the following:

$$\begin{aligned}
0 \leq D_{\overrightarrow{\mathbf{p}}}(\overrightarrow{\mathbf{Q}}) = \Bigg| & - \sum_{\overrightarrow{\mathbf{k}} \in FBZ} \left[J_{\overrightarrow{\mathbf{k}}} - J_{\overrightarrow{\mathbf{k}}+\overrightarrow{\mathbf{p}}}\right] \left\langle S^-_{\overrightarrow{\mathbf{k}}} S^+_{-\overrightarrow{\mathbf{k}}} + S^+_{\overrightarrow{\mathbf{k}}} S^-_{-\overrightarrow{\mathbf{k}}} + 4 S^z_{\overrightarrow{\mathbf{k}}} S^z_{-\overrightarrow{\mathbf{k}}} \right\rangle_{T,B,N} + \leq \\
& + \frac{2Bv_{cell}}{N} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N} \Bigg| \leq \Bigg| \sum_{\overrightarrow{\mathbf{k}} \in FBZ} \left[J_{\overrightarrow{\mathbf{k}}} - J_{\overrightarrow{\mathbf{k}}+\overrightarrow{\mathbf{p}}}\right] \left\langle S^-_{\overrightarrow{\mathbf{k}}} S^+_{-\overrightarrow{\mathbf{k}}} + S^+_{\overrightarrow{\mathbf{k}}} S^-_{-\overrightarrow{\mathbf{k}}} + 4 S^z_{\overrightarrow{\mathbf{k}}} S^z_{-\overrightarrow{\mathbf{k}}} \right\rangle_{T,B,N} \Bigg| + \\
& + \frac{2Bv_{cell}}{N} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N} \right| = F + \frac{2Bv_{cell}}{N} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N} \right|
\end{aligned} \tag{2.26}$$

The first term in (2.26) can be bounded as follows[5]:

$$\begin{aligned}
F = & \left| \sum_{\overrightarrow{\mathbf{k}} \in FBZ} \left[J_{\overrightarrow{\mathbf{k}}} - J_{\overrightarrow{\mathbf{k}}+\overrightarrow{\mathbf{p}}}\right] \left\langle S^-_{\overrightarrow{\mathbf{k}}} S^+_{-\overrightarrow{\mathbf{k}}} + S^+_{\overrightarrow{\mathbf{k}}} S^-_{-\overrightarrow{\mathbf{k}}} + 4 S^z_{\overrightarrow{\mathbf{k}}} S^z_{-\overrightarrow{\mathbf{k}}} \right\rangle_{T,B,N} \right| = \frac{1}{N^2} \left| \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) \times \right. \\
= & \left. \times \left[1 - e^{-i\overrightarrow{\mathbf{p}} \cdot \left(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1\right)}\right] \left\langle S^+(\overrightarrow{\mathbf{R}}_1) S^-(\overrightarrow{\mathbf{R}}_2) + S^-(\overrightarrow{\mathbf{R}}_1) S^+(\overrightarrow{\mathbf{R}}_2) + 4 S^z(\overrightarrow{\mathbf{R}}_1) S^z(\overrightarrow{\mathbf{R}}_2) \right\rangle \right| = \\
= & \frac{2}{N^2} \left| \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) \left[1 - \cos\left(\overrightarrow{\mathbf{p}} \cdot \left(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1\right)\right)\right] \left\langle \overrightarrow{S}(\overrightarrow{\mathbf{R}}_1) \cdot \overrightarrow{S}(\overrightarrow{\mathbf{R}}_2) + S^z(\overrightarrow{\mathbf{R}}_1) S^z(\overrightarrow{\mathbf{R}}_2) \right\rangle \right| \leq \\
\leq & \frac{1}{N^2} \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} \left| J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) \right| \left| \overrightarrow{\mathbf{p}} \cdot \left(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1\right) \right|^2 \left| \left\langle \overrightarrow{S}(\overrightarrow{\mathbf{R}}_1) \cdot \overrightarrow{S}(\overrightarrow{\mathbf{R}}_2) + S^z(\overrightarrow{\mathbf{R}}_1) S^z(\overrightarrow{\mathbf{R}}_2) \right\rangle \right| \leq \\
\leq & \frac{2}{N^2} \left| \overrightarrow{\mathbf{p}} \right|^2 \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} \left| J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) \right| \left| \overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1 \right|^2 \left| \left\langle \overrightarrow{S}(\overrightarrow{\mathbf{R}}_1) \cdot \overrightarrow{S}(\overrightarrow{\mathbf{R}}_2) \right\rangle \right| \leq \\
\leq & \frac{2S(S+1)}{N} \left| \overrightarrow{\mathbf{p}} \right|^2 \frac{1}{N} \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} \left| J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) \right| \left| \overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1 \right|^2 = \frac{1}{N} \Delta_N \left| \overrightarrow{\mathbf{p}} \right|^2
\end{aligned} \tag{2.27}$$

Where the parameter Δ_N is defined as:

$$\Delta_N = \frac{2S(S+1)}{N} \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} \left| J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) \right| \left| \overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1 \right|^2$$

.

Now, if the spin-spin couplings are short-ranged (i.e. $J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1)$ decays faster than $1/\left|\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1\right|^2$) then Δ_∞ is a finite quantity. At last, we can make use of the bound (2.27) to write the inequality (2.25) as follows:

[5] Here we make use of the following general result:

$$\sum_{\overrightarrow{\mathbf{k}}} J_{\overrightarrow{\mathbf{k}}+\overrightarrow{\mathbf{q}}} S^\alpha_{\overrightarrow{\mathbf{k}}} S^\beta_{-\overrightarrow{\mathbf{k}}} = \frac{1}{N^2} \sum_{\overrightarrow{\mathbf{R}}_1, \overrightarrow{\mathbf{R}}_2} J(\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1) S^\alpha(\overrightarrow{\mathbf{R}}_1) S^\beta(\overrightarrow{\mathbf{R}}_2) e^{-i\overrightarrow{\mathbf{q}} \cdot (\overrightarrow{\mathbf{R}}_2 - \overrightarrow{\mathbf{R}}_1)}$$

$$S(S+1) \geq \frac{4k_B T v_{cell}^2}{N} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle^2_{T,B,N} \left[\sum_{\overrightarrow{\mathbf{p}} \in FBZ} \frac{1}{\Delta_N \left| \overrightarrow{\mathbf{p}} \right|^2 + 2Bv_{cell} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N} \right|} \right] \tag{2.28}$$

In the thermodynamic limit, the sum in (2.28) can be replaced as an integral over the FBZ of the lattice, in the usual way — $\sum_{\overrightarrow{\mathbf{k}}} \to \frac{N v_{cell}}{(2\pi)^D} \int d^D \overrightarrow{\mathbf{k}}$:

$$S(S+1) \geq \frac{4k_B T v_{cell}^3}{(2\pi)^D} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle^2_{T,B,N} \int \frac{d^D \overrightarrow{\mathbf{p}}}{\Delta_N \left| \overrightarrow{\mathbf{p}} \right|^2 + 2Bv_{cell} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,N} \right|} \tag{2.29}$$

Finally, reaching the **Mermin-Wagner Inequality**, which survives even in the thermodynamic limit:

$$S(S+1) \geq \frac{4k_B T v_{cell}^3}{(2\pi)^D} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle^2_{T,B,\infty} \int \frac{d^D \overrightarrow{\mathbf{p}}}{\Delta_\infty \left| \overrightarrow{\mathbf{p}} \right|^2 + 2Bv_{cell} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} \tag{2.30}$$

2.2.2. Absence of order at $D = 1$ and $D = 2$

The Mermin-Wagner inequality — (2.30) — is not very useful, in general. But for one- and two-dimensional systems, after doing the integration, we will see that it can be used to prove that that $\left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right| = 0$,when $B \to 0$. As a consequence, these systems cannot be ordered at any finite temperature. Let us check both cases:

One-Dimensional Chain:

In this case, we have:

$$S(S+1) \geq \frac{4k_B T v_{cell}^3}{\Delta_\infty (2\pi)^D} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle^2_{T,B,\infty} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dp}{p^2 + \frac{2Bv_{cell}}{\Delta_\infty} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} \tag{2.31}$$

The integral in (2.31) is of the form — $\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dx}{x^2+A} = \frac{2 \arctan\left(\frac{\pi}{a\sqrt{A}}\right)}{\sqrt{A}}$. However, we do not worry about the complete form of the integral and maintain only a small-A approximation of it, which will be appropriate for taking the limit of vanishing external field. We have then:

$$S(S+1) \geq \frac{4k_B T v_{cell}^3}{\Delta_\infty (2\pi)} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle^2_{T,B,\infty} \frac{2\pi}{\sqrt{v_{cell} \frac{2Bv_{cell}}{\Delta_\infty} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|}} \iff$$

$$S(S+1) \geq k_B T a^{5/2} \sqrt{\frac{2}{\Delta_\infty B}} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|^{3/2} \tag{2.32}$$

And this means that:

$$0 \leq \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right| \leq \frac{\Delta_\infty^{1/3}}{a^{5/3}} \left(\frac{S(S+1)}{k_B T} \right)^{2/3} B^{1/3} \tag{2.33}$$

We then conclude that — $\lim_{B\to 0} \left[\lim_{N\to\infty} \left[\left\langle m^z(\overrightarrow{\mathbf{Q}}) \right\rangle_{T,B,N} \right] \right] = 0$ — ruling out any possibility for long-range order in a one-dimensional chain, at a finite temperature.

Two-Dimensional Lattice:

For a 2-D lattice, we have the slightly different integral:

$$S(S+1) \geq \frac{k_B T v_{cell}^3}{\Delta_\infty \pi^2} \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle^2_{T,B,\infty} \int\int_{FBZ} \frac{d^2 \overrightarrow{\mathbf{p}}}{\left| \overrightarrow{\mathbf{p}} \right|^2 + \frac{2Bv_{cell}}{\Delta_\infty} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} \tag{2.34}$$

Performing this integral analytically is not as straightforward as the last one (and it also depends on the details of the lattice), nevertheless we see that any eventual divergence will come from the long-wavelength sector of the FBZ. Hence we divide it into two parts - $\int_D + \int_{FBZ-D}$ - where D is a disk centered in the origin with a radius Λ (which is finite but can be taken arbitrarily small). The second integral is finite and positive for any value of $B \geq 0$, which corroborates our initial guess.

Meanwhile, the integral over D can be done in polar coordinates:

$$\int\int_D \frac{d^2 \overrightarrow{\mathbf{p}}}{\left| \overrightarrow{\mathbf{p}} \right|^2 + \frac{2Bv_{cell}}{\Delta_\infty} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} = 2\pi \int_0^\Lambda dp \frac{p}{p^2 + \frac{2Bv_{cell}}{\Delta_\infty} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} \tag{2.35}$$

The last integral is of the form $\int_0^\Lambda \frac{x dx}{x^2+A} = \frac{1}{2} \log \left[1 + \frac{\Lambda^2}{A} \right]$, which means that:

$$2\pi \int_0^\Lambda dp \frac{p}{p^2 + \frac{2Bv_{cell}}{\Delta_\infty} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} = \pi \log \left[1 + \frac{\Delta_\infty \Lambda^2}{2Bv_{cell} \left| \left\langle m^z_{\overrightarrow{\mathbf{Q}}} \right\rangle_{T,B,\infty} \right|} \right]$$

For small enough B, we have the following approximate form:

$$\pi \log\left[1+\frac{\Delta_\infty \Lambda^2}{2Bv_{cell}\left|\left\langle m^z_{\overrightarrow{\mathbf{Q}}}\right\rangle_{T,B,\infty}\right|}\right] \sim \pi\left[\log\left[\frac{\Delta_\infty \Lambda^2}{2v_{cell}\left|\left\langle m^z_{\overrightarrow{\mathbf{Q}}}\right\rangle_{T,B,\infty}\right|}\right]-\log\left[B\right]\right] \tag{2.36}$$

This can now be used to rewrite (2.34) as follows:

$$\begin{aligned} S(S+1) \geq \frac{k_B T v_{cell}^3}{\Delta_\infty \pi}\left\langle m^z_{\overrightarrow{\mathbf{Q}}}\right\rangle^2_{T,B,\infty}\left[(\text{finite})-\log\left[B\right]\right] \Longrightarrow \\ 0 \leq \left|\left\langle m^z_{\overrightarrow{\mathbf{Q}}}\right\rangle_{T,B,\infty}\right| \leq \sqrt{\frac{\Delta_\infty \pi}{k_B T v_{cell}^3}}\frac{1}{(\text{finite})-\log\left[B\right]} \end{aligned} \tag{2.37}$$

And obviously (2.37) means that $\lim_{B\to 0}\left[\lim_{N\to\infty}\left[\left\langle m^z(\overrightarrow{\mathbf{Q}})\right\rangle_{T,B,N}\right]\right]=0$ for any finite temperature, and any 2-dimensional Bravais Lattice.

2.2.3. The Mermin-Wagner Theorem

The conjunction of both these cases prove the Mermin-Wagner Theorem, which can be stated as follow:

Theorem 1 (Mermin-Wagner):

For the general Heisenberg Hamiltonian in a one- or two-dimensional Bravais lattice $\mathscr{L}$:

$$H_{Heis}=\sum_{\overrightarrow{\mathbf{R}}_1\in\mathscr{L}}\sum_{\overrightarrow{\mathbf{R}}_2\in\mathscr{L}} J\left(\overrightarrow{\mathbf{R}}_2-\overrightarrow{\mathbf{R}}_1\right)\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_1)\cdot\overrightarrow{\mathbf{S}}(\overrightarrow{\mathbf{R}}_2)-B\sum_{\overrightarrow{\mathbf{R}}_1\in\mathscr{L}} S^z(\overrightarrow{\mathbf{R}}_1)e^{-i\overrightarrow{\mathbf{Q}}\cdot\overrightarrow{\mathbf{R}}_1} \tag{2.38}$$

Such that the spin-spin interactions decay faster than $\frac{1}{\left|\overrightarrow{\mathbf{R}}_i-\overrightarrow{\mathbf{R}}_j\right|^2}$, there can be no spontaneous symmetry breaking at any finite temperature. I.e.

$$\lim_{B\to 0}\left[\lim_{N\to\infty}\left[\left\langle m^z(\overrightarrow{\mathbf{Q}})\right\rangle_{T,B,N}\right]\right]=0 \tag{2.39}$$

This theorem has a crucial importance in the current understanding of the phenomenon of symmetry breaking and not only in magnetic systems. In fact it had several generalizations over the years, either to other local Hamiltonians, other kinds of lattices, to the $T=0K$ regime and even to continuum models (in this context, it is usually referred as Coleman's Theorem). However, we will just stop on this stage, since it is this version that we really need to understand the results presented here.

2.3. Some Exact Statements About The AFM Ground State

In Chapter 1, we have seen that the exact ground-state of the Heisenberg AFM model is not known. Using approximate treatments (Spin-Wave Theory), we were able to study some properties of the ground-state, but those results are ever less reliable as the dimension of the system is decreased, becoming even useless for the one-dimensional chain. This realization may be despairing, but still there are some remarkable exact results that can be obtained about the ground-state and spectrum of the Heisenberg Model in a bipartite lattice. These results are obtained simply by using some symmetry considerations and clever mathematical tricks. In what follows some of these special theorems will be reviewed and proved.

2.3.1. Marshall's Theorem and Uniqueness of the Ground-State

References: [7,37]

In this subsection, we will prove two results about the ground-state of the Heisenberg AFM in a bipartite lattice. The first is called Marshall's Theorem and states that the lowest-energy state for each M-sector[6] of the Hilbert Space — $\mathscr{H}_{site}^{\otimes N}$ — of Heisenberg Model is unique and can be expanded in the product basis, with only real coefficients, obeying a simple sign criterion:

Theorem 1 (Marshall's Theorem)

If one considers a given sector of $\mathscr{H}_{site}^{\otimes N}$ labeled by $M = \sum_{i\in\mathscr{L}} m_i$, the lowest-energy eigenstate of H_{Heis} in this sector is non-degenerate and can be written as:

$$\left|\Psi_0^M\right\rangle = \sum_{\alpha}(-1)^{\sum_{i\in\mathscr{L}_B}(s+m_i^\alpha)} f_\alpha^M \left|\phi_\alpha\right\rangle$$

Where the sum is only over the product states $|\phi_\alpha\rangle$ that have $\sum_i m_i = M$ and f_α^M are positive real numbers.

With Marshall's Theorem, we manage to reduce the number of candidates for the ground-state of the Heisenberg AFM, to a total of $2N+1$ different states (one for each M-sector). However, we will also be able to prove a second important result which tells us that the exact ground-state of this model is unique and a singlet of the total spin operator[7]:

[6] As was already commented in the beginning of the chapter (and proved in the Appendix 2A), the Hamiltonian H_{Heis} is invariant under space rotations, meaning that its eigenstates can be chosen to be of the form $|S_{tot}, M\rangle$, which naturally breaks the total Hilbert Space into M sectors. If the number of spins is even, then - $M \in \{-Ns, -Ns+1, ..., -1, 0, 1, ..., Ns-1, Ns\}$.

Furthermore, by symmetry it is clear that the energy of the eigenstates can only be a function of S_{tot}, and never of M.

[7] This last statement may sound like a complete characterization of the true ground-state. However, we must remind the reader that there is a macroscopic number of global spin singlets, for a macroscopic lattice of spins!

Theorem 2 (Uniqueness and Isotropy of the Ground State):

The absolute ground-state of the AFM model in a bipartite lattice with equal size sublattices[a] (consequently an even number of spins) is unique and a singlet of the total spin, i.e.:

$$S^2_{Tot}\left|GS\right\rangle = 0$$

[a]The problem with our proof actually arises only when there is an odd number of spins in the system, since a singlet state does not exist. In this case, we have:

$$S^2_{Tot}\left|GS\right\rangle = s(s+1)\left|GS\right\rangle$$

Which also has a null magnetization in the thermodynamic limit.

The proof of both results was first done in Ref. [37], but our detailed proof is based in the book [7]. Before embarking into the proof of these results, we shall start by establishing some useful conventions:

Conventions and definitions:

The Hilbert Space associated to the Heisenberg AFM model in a lattice with N cells is just $\mathscr{H}_{site}^{\otimes N}$, where $\mathscr{H}_{site}$ is the $(2s+1)$-dimensional Hilbert space spanned by the basis $\left|s,m_i\right\rangle_i$ [with $m_i \in \{-s,-s+1,...,s-1,s\}$]. An orthonormal basis for this space could be chosen as usual - $\left|\phi_\alpha\right\rangle = \left[\underset{i\in\mathscr{L}_A}{\otimes}\left|s,m_i^\alpha\right\rangle_i\right]\left[\underset{j\in\mathscr{L}_B}{\otimes}\left|s,m_j^\alpha\right\rangle_j\right]$.

However, for our purposes is convenient to do an unitary transformation on these states and write everything in terms of the new basis (2.40)[8]:

$$\left|\widetilde{\phi}_\alpha\right\rangle = \left[\underset{i\in\mathscr{L}_A}{\otimes}\left|s,m_i^\alpha\right\rangle_i\right]\left[\underset{j\in\mathscr{L}_B}{\otimes}(-1)^{s+m_j^\alpha}\left|s,m_j^\alpha\right\rangle_j\right] \tag{2.40}$$

In this basis, the Marshall's sign criterion is trivial — i.e. all of the coefficients are positive numbers. We can also calculate the matrix elements of H_{Heis} :

$$\left\langle\widetilde{\phi}_\beta\right| H_{Heis}\left|\widetilde{\phi}_\alpha\right\rangle = \frac{J}{2}\sum_{bonds}\left\langle\widetilde{\phi}_\beta\right|\left[\frac{1}{2}\left\{S_i^+S_j^- + S_i^-S_j^+\right\} + S_i^zS_j^z\right]\left|\widetilde{\phi}_\alpha\right\rangle \tag{2.41}$$

For a product basis like (2.40) we have $\left\langle\widetilde{\phi}_\beta\right|\frac{J}{2}\sum_{bonds}S_i^zS_j^z\left|\widetilde{\phi}_\alpha\right\rangle = \lambda_\alpha\delta_{\alpha\beta}$, so it remains only to calculate the terms like in (2.42) (where i and j are first neighbors). These either give 0 or the following:

[8]This is obviously a unitary transformation, since in each local Hilbert space $\mathscr{H}_{site\,i}$, the matrix U_i (that implements the transformation) is of the form $diag\,(1-11-1...)$, thus being unitary. For the whole space, we just take $U=\oplus_i U_i$ which inherits unitarity.

$$
\begin{aligned}
S^-_{i\in\mathscr{L}_A} S^+_{j\in\mathscr{L}_B} \left|\widetilde{\phi}_\alpha\right\rangle &= ... \otimes S^-_i \left|s, m^\alpha_i\right\rangle_i \otimes ... \otimes (-1)^{s+m^\alpha_j} S^+_j \left|s, m^\alpha_j\right\rangle_j \otimes ... \\
&= -\sqrt{(s(s+1) - m^\alpha_i(m^\alpha_i - 1))\left(s(s+1) - m^\alpha_j(m^\alpha_j - 1)\right)} \times \\
&\times \left[... \otimes \left|s, m^\alpha_i - 1\right\rangle_i \otimes ... \otimes (-1)^{s+m^\alpha_j+1} \left|s, m^\alpha_j + 1\right\rangle_j \otimes ...\right]
\end{aligned} \tag{2.42}
$$

The last result means that there is only one basis state whose matrix element of $S^-_{i\in\mathscr{L}_A} S^+_{j\in\mathscr{L}_B}$ with $\left|\widetilde{\phi}_\alpha\right\rangle$ is nonzero. In that case, the matrix element is therefore negative. Hence, we can write the general expression (2.43), stating the non-negativity of the the matrix elements for the non-diagonal part of H_{Heis}.

$$
\left\langle\widetilde{\phi}_\beta\right| \left[\frac{J}{4} \sum_{bonds} \left\{S^+_i S^-_j + S^-_i S^+_j\right\}\right] \left|\widetilde{\phi}_\alpha\right\rangle = -\left|K_{\beta\alpha}\right| \tag{2.43}
$$

Proof of Marshall's Theorem (Theorem 1):

- **Motivation:**

The expression (2.43) allow us to prove our first important theorem — Marshall's Theorem. The proof is divided in two parts:

1. First, we must prove that a ground-state of an M-sector satisfies the sign criterion. The main idea of this proof is to expand a ground-state of an M-sector in terms of the new basis — $\left|\Psi^M_0\right\rangle = \sum_\alpha f^M_\alpha \left|\widetilde{\phi}_\alpha\right\rangle$ — and then use (2.43) to write the corresponding Schrodinger Equation. Using this equation and the negativity of the matrix elements (2.43), we can prove that $f^M_\alpha \geq 0$. The case $f^M_\alpha = 0$ is also ruled out by a simple contradiction argument.
2. Secondly, we have to show that the ground-state $\left|\Psi^M_0\right\rangle$ is unique in that M-sector. To do that, we will proceed by contradiction, by assuming that there is another ground-state orthogonal to it, and then use the sign criterion to arrive at a contradiction.

Let us now proceed with the formal proof.

- **Formal Proof:**

We start by writing the Schrödinger equation for a general state in the M-sector - $\left|\Psi^M\right\rangle$ - using the $\left|\widetilde{\phi}_\alpha\right\rangle$ representation - $\left|\Psi^M\right\rangle = \sum_\alpha f^M_\alpha \left|\widetilde{\phi}_\alpha\right\rangle$. The coefficients of this expansion can be chosen as real numbers[9].

[9] An hand-waving (but good and simple) argument for this is the following: If $\left|\Psi^M\right\rangle$ is an eigenstate of H_{Heis}, it is one of the states $|S_{tot}, M\rangle$ and since those are linear combinations of product states with coefficients that are products of Clebsh-Gordan coefficients, they are real numbers.

$$\left\langle \widetilde{\phi}_\beta \right| H_{Heis} \left|\Psi^M\right\rangle = E \left\langle \widetilde{\phi}_\beta \mid \Psi^M \right\rangle \Leftrightarrow \lambda_\beta f_\beta^M - \sum_\alpha |K_{\beta\alpha}| \, f_\alpha^M = E f_\beta^M \tag{2.44}$$

Now, we will choose the coefficients f_α^M such that $\left|\Psi^M\right\rangle$ is a ground-state of the M-sector (with energy E_0^M), designating it as $\left|\Psi_0^M\right\rangle$. Furthermore, we can consider a different state defined as follows:

$$\left|\overline{\Psi}_0^M\right\rangle = \sum_\alpha \left|f_\alpha^M\right| \left|\widetilde{\phi}_\alpha\right\rangle \tag{2.45}$$

Calculating the energy expectation value for the state (2.45), we get the trivial inequality (2.46).

$$\begin{aligned} \left\langle \overline{\Psi}_0^M \right| H_{Heis} \left|\overline{\Psi}_0^M\right\rangle &= \sum_\beta \lambda_\beta \left|f_\beta^M\right|^2 - \sum_{\alpha\beta} |K_{\beta\alpha}| \left|f_\alpha^M\right| \left|f_\beta^M\right| \leq \\ &\leq \sum_\beta \lambda_\beta \left|f_\beta^M\right|^2 - \sum_{\alpha\beta} |K_{\beta\alpha}| \, f_\alpha^M f_\beta^M = E_0^M \end{aligned} \tag{2.46}$$

This means that $\left|\overline{\Psi}_0^M\right\rangle$ is also a ground-state of the M-sector.

Finally, it remains to be shown that $f_\alpha^M = \left|f_\alpha^M\right|, \forall\alpha \Longrightarrow \left|\Psi_0^M\right\rangle = \left|\overline{\Psi}_0^M\right\rangle$. For that, we take advantage of the fact that $\lambda_\beta - E_0 = \frac{1}{\left|f_\beta^M\right|} \sum_\alpha |K_{\beta\alpha}| \left|f_\alpha^M\right| \geq 0$[10] and write:

$$\begin{aligned} \left(\lambda_\beta - E_0^M\right) f_\beta^M = \sum_\alpha |K_{\beta\alpha}| \, f_\alpha^M \Rightarrow \left(\lambda_\beta - E_0^M\right) \left|f_\beta^M\right| &= \left| \sum_\alpha |K_{\beta\alpha}| \, f_\alpha^M \right| \\ \Rightarrow \sum_\alpha |K_{\beta\alpha}| \left|f_\alpha^M\right| &= \left| \sum_\alpha |K_{\beta\alpha}| \, f_\alpha^M \right| \end{aligned} \tag{2.47}$$

But the equality (2.47) can only be true if $f_\alpha^M \geq 0$, for all α!As as matter of fact, the null case is also excluded by the following argument by *reductio ad absurdum*:

For any given $\left|\widetilde{\phi}_\beta\right\rangle$, there is at least one other $\left|\widetilde{\phi}_\alpha\right\rangle$ in the same M-sector such that $|K_{\beta\alpha}| \neq 0$. Then, let us suppose that a given $f_\alpha^M = 0$, then the equation (2.44) yields the following result:

$$\sum_\alpha |K_{\beta\alpha}| \, f_\alpha^M = 0$$

But this is a contradiction, because each of the terms in the sum (of positive numbers) is non-null. This means that, if one of the coefficients is null, all the others are also.

[10] This is a direct consequence of equation (2.44) and the fact that E_0 is the ground-state energy.

The final conclusion is that $f_\alpha^M > 0$. When we rewrite the definition of $\left|\Psi_0^M\right\rangle$ to the original product basis $|\phi_\alpha\rangle$, we get the intended result:

$$\left|\Psi_0^M\right\rangle = \sum_\alpha (-1)^{\sum_{i\in\mathscr{L}_B}(s+m_i^\alpha)} f_\alpha^M \left|\phi_\alpha\right\rangle \tag{2.48}$$

At last, to prove that $\left|\Psi_0^M\right\rangle$ is the unique ground state of the M-sector, we assume that there is another ground-state $\left|\chi_0^M\right\rangle = \sum_\alpha g_\alpha^M \left|\widetilde{\phi}_\alpha\right\rangle$ (where $g_\alpha^M > 0$ as before), which is orthogonal to $\left|\Psi_0^M\right\rangle$.

Then, by calculating the braket $\left\langle\chi_0^M \mid \Psi_0^M\right\rangle$, we arrive at the following conclusion:

$$\left\langle\chi_0^M \mid \Psi_0^M\right\rangle = \sum_\alpha g_\alpha^M f_\alpha^M > 0 \tag{2.49}$$

And this is contradicting the assumed orthogonality between the states. Hence, the two states must be the same and this completes de proof of Marshall's Theorem.

□

Proof of the Uniqueness and Isotropy of the Ground-State (Theorem 2):

- **Motivation:**

Building on the ideas of the last proof, we know that by symmetry, the energy of a state — $|S_{Tot}, M, ...\rangle$ — does not depend on the M quantum number, but it will depend on $0 \leq S_{Tot} \leq Ns$. The secret for proving this theorem is to check what if the energy increases or decreases with S_{Tot} in each of the M-sectors. This is done by:

1. First, comparing the Heisenberg Model with the exactly soluble Infinite-Range Quantum Antiferromagnet (IRQAFM), to which Marshall's Theorem also applies. From the spectrum of this model, we conclude that the ground-state of an M-sector is a state with lowest possible S_{Tot}, .i.e. $S_{Tot} = |M|$.
2. Using the invariance of the energy with M, we are able to conclude that the absolute ground-state will be the ground-state of the 0-sector, and hence a singlet.

We proceed with the formal proof of this Theorem:

- **Formal Proof:**

We start by defining the Infinite-Range Quantum Antiferromagnet (IRQAFM) in (2.50). This $O(3)$-invariant model also lives in a bipartite lattice of spins with the following Hamiltonian:

$$H_{IRQAFM} = J \sum_{i \in \mathscr{L}_A} \sum_{j \in \mathscr{L}_B} \overrightarrow{S}_i \cdot \overrightarrow{S}_j \quad with\ J > 0 \tag{2.50}$$

This model is solved in [Appendix B.2] and its eigenstates are found to be of the form $|S_{tot}, M; S_{TotA}, S_{TotB}\rangle$ [11]. The spectrum of the model is given in equation (2.51).

$$E_\infty(S_{tot}, S_{TotA}, S_{TotB}) = \frac{J}{2}\left[S_{tot}\left(S_{tot}+1\right) - S_{totA}\left(S_{totA}+1\right) - S_{totB}\left(S_{totB}+1\right)\right] \tag{2.51}$$

In this soluble case, we can see that, in each M-sector, the energy is minimized by the state with $S_{totA} = S_{totB} = \frac{Ns}{2}$ and $S_{tot} = |M|$. This means that the M-sector's lowest-energy state - $\left|\Psi_\infty^M\right\rangle$ - obeys $S_{Tot}^2\left|\Psi_\infty^M\right\rangle = |M|\left(|M|+1\right)\left|\Psi_\infty^M\right\rangle$.

Since (2.50) also obeys Marshall's Theorem, we can write — $\left|\Psi_\infty^M\right\rangle = \sum_\alpha (-1)^{\sum_{\mathscr{L}_B}(s+m_i^\alpha)}\, g_\alpha^M \left|\widetilde{\phi}_\alpha\right\rangle$ — and its overlap with the M-sector ground-state of the corresponding Heisenberg model is:

$$\left\langle \Psi_\infty^M \mid \Psi_0^M \right\rangle = \sum_\alpha g_\alpha^M f_\alpha^M \neq 0 \tag{2.52}$$

Both $\left|\Psi_\infty^M\right\rangle$ and $\left|\Psi_0^M\right\rangle$ are eigenstates of the total spin operator S_{Tot}^2 and by (2.52), they must share the same total spin quantum number[12]. Hence, we conclude that:

$$S_{Tot}^2\left|\Psi_0^M\right\rangle = |M|\left(|M|+1\right)\left|\Psi_0^M\right\rangle$$

In particular, this means that the unique ground-state of the 0-sector is a singlet state. To see that this is also the global ground-state, we just notice that the energy does not depend on M and that each M-sector is spanned by states of the form $|S_{tot}, M, ...\rangle$, with $S_{tot} \geq M$. Furthermore, it is also obvious that each of the total spins — $1 \leq S_{tot} \leq Ns$ — is represented in more than one M-sector, their eigenenergies being equal to E_0^M, for some $M \neq 0$. Therefore, we conclude that:

$$E_0^M \geq E_0^{M=0} \quad for \quad all \quad M$$

Which completes the proof of the Theorem 2.

□

2.3.2. The Lieb-Schultz-Mattis Theorem for 1-D AFM Heisenberg Chain

References: [6,7,9]

[11] Where S_{TotA} and S_{TotB} are the total spin quantum numbers of each of the sublattices [S_{TotA}, $S_{TotB} \in \{0, ..., \frac{Ns}{2}\}$]
[12] Because this is a good quantum number.

In this subsection, we will proceed by proving a very important result about the low-energy spectrum for 1-dimensional AFM Heisenberg chain with half-integer on-site spins. This result was first proved in [9] stands as follows:

Theorem 3 (Lieb-Schultz-Mattis Theorem for the 1-D chain):

For the half-integer spin Heisenberg chain with periodic boundary conditions, given by the Hamiltonian:

$$H_{Heis}(N) = J\sum_{j=1}^{N-1}\left[1/2\left\{S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right\} + S_j^zS_{j+1}^z\right] + J\left[1/2\left\{S_N^+S_1^- + S_N^-S_1^+\right\} + S_N^zS_1^z\right]$$

There are gapless excitations above the ground-state, in the thermodynamic limit — $N \to +\infty$ (in even steps).[a]

[a] In this case we are taking the thermodynamic limit as the limit of a succession of Heisenberg chains with an even number of sites and respecting periodic boundary conditions.

Proof of the LST Theorem:

- **Motivation:**

The proof is of this theorem is done by explicit construction of a state orthogonal to the ground-state, that is shown to have an energy which goes to E_0 in the limit of large N. Our procedure will the same as used in [6,9], starting by defining **Twisting Operator** as:

$$\mathcal{O}^1 = \prod_{j=1}^{N}\exp\left(i\frac{2\pi}{N}jS_j^z\right) \tag{2.53}$$

Where the exponentials in (2.53) are rotation operators of individual spins, by an angle of $2\pi j/N$ radians about the z-axis. This action is represented in Figure 2.1.

If we denote the unique ground-state of the AFM model by $|\Psi_0\rangle$, our gapless excited state is defined by acting with a twist on it —$|\Psi_1\rangle = \mathcal{O}^1|\Psi_0\rangle$. The heart of the proof is now to show that, as $N \to \infty$, the energy expectation value of $|\Psi_1\rangle$ will tend to E_0, and also to check that $\langle\Psi_0 \mid \Psi_1\rangle = 0$. This last step will be only possible for the case when the local spins are half-integers, thanks to the non trivial phase acquired in a 2π rotation.

- **Formal Proof:**

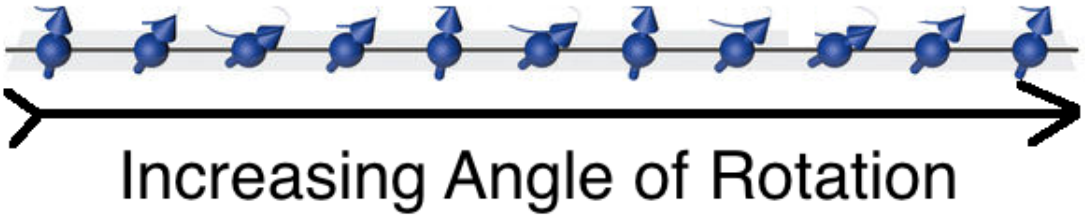


Figure 2.1.: Pictorial representation of the transformation implemented by the 'twisting operator' - $\mathcal{O}^1$ - in a spin chain.

Taking over the definitions given above, we have no reason to think that $|\Psi_1\rangle$ is an eigenstate of H_{Heis}. However, we can still calculate the expectation value for energy associated with it. We leave the detailed calculations for [Appendix B.3], but the result is the following:

$$\begin{aligned}
&\langle\Psi_1| H_{Heis} |\Psi_1\rangle = \langle\Psi_0| \mathcal{O}^{1\dagger} H_{Heis} \mathcal{O}^1 |\Psi_0\rangle = \\
&= E_0 + \frac{J}{2}\sum_{j=1}^{N-1}\left[\left(e^{i\frac{2\pi}{N}}-1\right)\langle\Psi_0| S_j^+ S_{j+1}^- |\Psi_0\rangle + \left(e^{-i\frac{2\pi}{N}}-1\right)\langle\Psi_0| S_j^- S_{j+1}^+ |\Psi_0\rangle\right] \\
&+ \frac{J}{2}\left[\left(e^{-i\frac{2\pi}{N}}-1\right)\langle\Psi_0| S_N^+ S_1^- |\Psi_0\rangle + \left(e^{i\frac{2\pi}{N}}-1\right)\langle\Psi_0| S_N^- S_1^+ |\Psi_0\rangle\right]
\end{aligned} \tag{2.54}$$

We can now find a precise bound for $\langle\Psi_0| S_i^{\pm} S_j^{\mp} |\Psi_0\rangle$, by noticing that:

$$\begin{aligned}
\langle\Psi_0| S_i^{\pm} S_j^{\mp} |\Psi_0\rangle &= \langle\Psi_0| (S_i^x \pm i S_i^y)(S_j^x \mp i S_j^y) |\Psi_0\rangle = \\
&= \langle\Psi_0| S_i^x S_j^x + S_i^y S_j^y |\Psi_0\rangle \pm i \langle\Psi_0| S_i^y S_j^x - S_i^x S_j^y |\Psi_0\rangle
\end{aligned}$$

Which yields[13]:

$$\langle\Psi_0| S_i^{\pm} S_j^{\mp} |\Psi_0\rangle = \langle\Psi_0| S_i^x S_j^x + S_i^y S_j^y |\Psi_0\rangle \leq 2s^2 \tag{2.55}$$

Applying inequality (2.55) to (2.54), we get the following result:

$$\langle\Psi_1| H_{Heis} |\Psi_1\rangle \leq E_0 + 4JNs^2(\cos\left(\frac{2\pi}{N}\right) - 1) \sim E_0 + \frac{8\pi J s^2}{N} + \mathcal{O}\left(N^{-3}\right) \tag{2.56}$$

In the thermodynamic limit, this yields $\lim_{N\to\infty}\left[\langle\Psi_1| H_{Heis} |\Psi_1\rangle - E_0\right] = 0$.

The only thing that remains to be proven is that $|\Psi_1\rangle$ is orthogonal to the unique ground-state of the system. i.e. that $\langle\Psi_0 \mid \Psi_1\rangle = 0$. To do that, we use explicitly the lattice translation invariance of the

[13]Note that the term $\langle\Psi_0| S_i^y S_j^x - S_i^x S_j^y |\Psi_0\rangle$ is null by symmetry. Since the ground state is invariant under rotations, we can write $e^{i\pi S_{tot}^z} |\Psi_0\rangle = |\Psi_0\rangle$, which means that $\langle\Psi_0| S_i^y S_j^x - S_i^x S_j^y |\Psi_0\rangle = \langle\Psi_0| e^{-i\pi S_{tot}^z}\left(S_i^y S_j^x - S_i^x S_j^y\right) e^{i\pi S_{tot}^z} |\Psi_0\rangle = -\langle\Psi_0| S_i^y S_j^x - S_i^x S_j^y |\Psi_0\rangle$, meaning that it must be zero.

ground-state[14].

Defining the primitive lattice translation operator - U_a - as:

$$[U_a, H_{Heis}] = 0; \quad U_a^\dagger \overrightarrow{S}_i U_a = \overrightarrow{S}_{i+1}; \quad U_a^\dagger \overrightarrow{S}_N U_a = \overrightarrow{S}_1 \tag{2.57}$$

Such that $U_a |\Psi_0\rangle = |\Psi_0\rangle$. In the end, we wish to calculate $\langle \Psi_0 \mid \Psi_1 \rangle$, as follows:

$$\begin{aligned}
\langle \Psi_0 \mid \Psi_1 \rangle = \langle \Psi_0 | \mathcal{O}^1 | \Psi_0 \rangle = \langle \Psi_0 | U_a^\dagger \mathcal{O}^1 U_a | \Psi_0 \rangle = \langle \Psi_0 | \prod_{j=1}^{N} \left[U_a^\dagger \exp\left(i \frac{2\pi}{N} j S_j^z \right) U_a \right] | \Psi_0 \rangle = \\
= \langle \Psi_0 | \prod_{j=2}^{N} \left[\exp\left(i \frac{2\pi}{N} (j-1) S_j^z \right) \right] \exp\left(2\pi i S_1^z \right) | \Psi_0 \rangle = \\
= \langle \Psi_0 | \prod_{j=1}^{N} \left[\exp\left(i \frac{2\pi}{N} (j-1) S_j^z \right) \right] \exp\left(2\pi i S_1^z \right) | \Psi_0 \rangle = \\
= \langle \Psi_0 | \prod_{j=1}^{N} \left[\exp\left(i \frac{2\pi}{N} j S_j^z \right) \right] \exp\left(-i \frac{2\pi}{N} S_{Tot}^z \right) \exp\left(2\pi i S_1^z \right) | \Psi_0 \rangle = \\
= \langle \Psi_0 | \mathcal{O}^1 \exp\left(-i \frac{2\pi}{N} S_{Tot}^z \right) \exp\left(2\pi i S_1^z \right) | \Psi_0 \rangle
\end{aligned} \tag{2.58}$$

Since $\exp\left(2\pi i S_1^z\right) |\Psi_0\rangle = \sum_\alpha f_\alpha \exp\left(2\pi i S_1^z\right) |s, m_\alpha\rangle_1 \otimes ... = \pm |\Psi_0\rangle$, where the $+$ refers to the case where s is an integer and the $-$ to the half-integer case.

In the case of the Heisenberg Model the ground-state is a global singlet, which guarantees that $\exp\left(-i\frac{2\pi}{N} S_{Tot}^z\right) |\Psi_0\rangle = |\Psi_0\rangle$. This yields the following result:

$$\langle \Psi_0 \mid \Psi_1 \rangle = \begin{cases} \langle \Psi_0 \mid \Psi_1 \rangle & s\ integer \\ -\langle \Psi_0 \mid \Psi_1 \rangle & s\ half-integer \end{cases} \tag{2.59}$$

As a conclusion from (2.59) is that, in the case where $s = 1/2, 3/2, 5/2, ...$, the twisted state $|\Psi_1\rangle$ is orthogonal to the ground-state.

2.3.3. Generalization of the LSM Theorem to Higher-Dimensional Cubic Lattices

The above construction can be applied equally well to higher-dimensional lattices, as was already suggested in the original article [9]. The main idea of this generalization is to choose one of the basis vectors of the underlying Bravais lattice and define a **Twisting Operator** — $\mathcal{O}^d$ —that does exactly the same as $\mathcal{O}^1$, but with the rotation angle increasing only in the chosen direction.

To see how that is done, we will take up the case of an $N_x \times N_y$ square lattice (with PBC), whose Heisenberg Hamiltonian can be easily written as:

[14] If the reader is wondering about a possible breaking of translation invariance in the ground-state, it may be worth reminding that if there was such a breaking of translation symmetry, the ground-state could not be unique. Acting with the translation operator on $|\Psi_0\rangle$ would generate another ground-state, orthogonal to it. Therefore, in a system with a unique ground-state, the ground-state is always invariant under all the symmetry operations that leave the Hamiltonian invariant.

$$H^{Sq}_{Heis} = J \sum_{n=1}^{N_x-1} \sum_{m=1}^{N_y-1} [1/2 \left\{ S^+_{n,m} S^-_{n+1,m} + S^+_{n,m} S^-_{n,m+1} + S^-_{n,m} S^+_{n+1,m} + S^-_{n,m} S^+_{n,m+1} \right\} + S^z_{n,m} S^z_{n+1,m} + S^z_{n,m} S^z_{n,m+1}] + (\textit{boundary couplings}) \tag{2.60}$$

The labels $(n, m) \in \mathscr{L}_{Sq}$ are integers that name all the sites in the square lattice. Now, we introduce the x**-direction Twisting Operator** - $\mathcal{O}^2$:

$$\mathcal{O}^2 = \prod_{n=1}^{N_x} \prod_{m=1}^{N_y} \exp\left(i \frac{2\pi}{N} n S^z_{n,m} \right) \tag{2.61}$$

As was done in one-dimensional case, we see that the following general result is true (for any two sites (n, m) and (l, k)):

$$\mathcal{O}^{2\dagger} \left[S^+_{n,m} S^-_{l,k} + S^-_{n,m} S^+_{l,k} \right] \mathcal{O}^2 = \left(e^{i \frac{2\pi}{N}(n-l)} \right) S^+_{n,m} S^-_{l,k} + \left(e^{-i \frac{2\pi}{N}(n-l)} \right) S^-_{n,m} S^+_{l,k} \tag{2.62}$$

Applying (2.62) to the Hamiltonian (2.60), one gets:

$$\mathcal{O}^{2\dagger} H^{Sq}_{Heis} \mathcal{O}^2 = H^{Sq}_{Heis} + \frac{J}{2} \sum_{n=1}^{N_x-1} \sum_{m=1}^{N_y-1} \left[\left(e^{i \frac{2\pi}{N}} - 1 \right) S^+_{n,m} S^-_{n+1,m} + \left(e^{-i \frac{2\pi}{N}} - 1 \right) S^-_{n,m} S^+_{n+1,m} \right] + (\textit{boundary terms}) \tag{2.63}$$

From here on, the procedure to build the a gapless state is similar to the former case. We define $|\Psi_2\rangle = \mathcal{O}^2 |\Psi_0\rangle$, where $|\Psi_0\rangle$ is the unique ground-state of the model.

To prove that $\langle \Psi_0 \mid \Psi_2 \rangle = 0$, we resort again to translation symmetry in the x-direction, implemented by the unitary operator U_{a_x} (such that $U_{a_x} |\Psi_0\rangle = |\Psi_0\rangle$). This means that:

$$\begin{aligned}
\langle \Psi_0 \mid \Psi_2 \rangle &= \langle \Psi_0 | \mathcal{O}^2 | \Psi_0 \rangle = \langle \Psi_0 | U^\dagger_{a_x} \mathcal{O}^2 U_{a_x} | \Psi_0 \rangle = \langle \Psi_0 | \prod_{m=1}^{N_x} \prod_{n=1}^{N_y} \left[U^\dagger_{a_x} \exp\left(i \frac{2\pi}{N} n S^z_{n,m} \right) U_a \right] | \Psi_0 \rangle = \\
&= \langle \Psi_0 | \prod_{m=1}^{N_y} \left\{ \prod_{n=2}^{N_x} \left[\exp\left(i \frac{2\pi}{N} (n-1) S^z_{n,m} \right) \right] \exp\left(2\pi i S^z_{1,m} \right) \right\} | \Psi_0 \rangle = \\
&= \langle \Psi_0 | \prod_{m=1}^{N_y} \left\{ \prod_{n=1}^{N_x} \left[\exp\left(i \frac{2\pi}{N} (n-1) S^z_{n,m} \right) \right] \exp\left(2\pi i S^z_{1,m} \right) \right\} | \Psi_0 \rangle = \\
&= \langle \Psi_0 | \prod_{m=1}^{N_y} \left\{ \prod_{n=1}^{N_x} \left[\exp\left(i \frac{2\pi}{N} n S^z_{n,m} \right) \right] \exp\left(2\pi i S^z_{1,m} \right) \right\} \exp\left(-i \frac{2\pi}{N} S^z_{Tot} \right) | \Psi_0 \rangle = \\
&= \langle \Psi_0 | \mathcal{O}^2 \prod_{m=1}^{N_y} \left[\exp\left(2\pi i S^z_{1,m} \right) \right] | \Psi_0 \rangle
\end{aligned} \tag{2.64}$$

If we assume that N_y is an odd-integer[15] and the local spins are half-integer multiplets, we have:

$$\prod_{m=1}^{N_y} \left[\exp\left(2\pi i S^z_{1,m}\right)\right] |\Psi_0\rangle = -|\Psi_0\rangle$$

And, consequently, $\langle\Psi_0 \mid \Psi_2\rangle = -\langle\Psi_0 \mid \Psi_2\rangle = 0$.

Finally, it can be proven that $\lim_{N\to\infty}\left[\langle\Psi_2| H_{Heis} |\Psi_2\rangle - E_0\right] = 0$, by picking up equation (2.63) and making the same approximations done in the one-dimensional case. This yields the following:

$$\langle\Psi_2| H^{Sq}_{Heis} |\Psi_2\rangle = \langle\Psi_0| \mathcal{O}^{2\dagger} H^{Sq}_{Heis} \mathcal{O}^2 |\Psi_0\rangle = E_0 + \mathcal{O}\left(\frac{1}{N}\right) \tag{2.65}$$

The generalization of this result to any d-dimensional Bravais lattices is trivial, being only a question of writing out all the terms in the Hamiltonian like we did in (2.60). Hence, the half-integer Heisenberg Model is always gapless!

2.4. Preliminary Conclusions and Open Questions

The importance of the Heisenberg model, for our understanding of physical phenomena, rests mostly on its ability to predict magnetic order (FM or AFM). Our first approach - Spin-Wave Theory - allowed us to obtain some useful results concerning the structure of the ground-state and low-energy excited states, but still our calculations were filled with ill-defined expressions and dubious definitions. A partial explanation for those problems was found in this chapter, by the realization that a finite temperature magnetic long-range order is not possible for this model in low-dimensional spaces ($d = 1, 2$). Nevertheless, the physics is not exhausted by the absence of order, and many questions regarding the true spectrum of these models, especially when talking about the $T = 0$ regime (where the Mermin-Wagner Theorem does not apply).

To address that problem, we have proven two very important rigorous theorems about the Heisenberg AFM Models:

1. The Ground-State is always unique and a singlet of total lattice spin;
2. If the local spins are half-integers, the low-energy spectrum is gapless;

The first result is surprising and is a statement of the great complexity of the exact ground-state associated to this model. In fact, one can see that if there is symmetry breaking in this model, it will be of a nature very different from the corresponding FM model. As discussed by P. W. Anderson

[15] Obviously, this assumption requires a comment. It seems that we are considering a very particular case, by taking N_y to be odd. However, we usually assume that, in the thermodynamic limit, the physics of the model won't be heavily influenced by adding or removing one line of spins. Therefore, our claim is that this theorem is still valid in the general case, although its proof is not.

[2,5], the long-lasting order in the AFM is a consequence of the fact that, in the thermodynamic limit, magnetized states are energetically close to the (isotropic) ground-state, such that the time needed for the magnetization to shift direction is infinite. Obviously, this insight indicates that, at $T = 0$, a very relevant question to ask is if the model has a gap above the ground-state or not. If it is gapped, then it will be disordered (this is discussed rigorously in [7]).

This question was settled for the case where then localized spins are half-integers, where we were able to prove that all such models are gapless and can, in principle, hold Neél order. However, for the integer spin cases, nothing could be said, and for $d = 1$, not even the spin-wave calculations were able to yield comprehensible results. The treatment of those cases will require the use of field-theoretical tools, and will be the main theme for the next chapter.

3. Path-Integral Formulation of the Heisenberg Model

As remarked in the end of last chapter, we are to build a new formalism that help us dealing with the Heisenberg AFM Model without having to assume a magnetized state. That requires us to rephrase those models in terms of path-integrals, in which all physical quantities of interest (namely correlation functions) can be computed by summing over all the possible spin configurations in the system.

Most people are familiar with this approach in the context of the single-particle quantum mechanics, where the state of the system is represented by a point in phase space $(\mathbf{q}, \mathbf{p})$. This formalism is also commonly known, in the case of continuous Quantum Field Theory, where a value of the field is attributed to each point in space-time. However, in either case, the state of the system can be labeled by a set of continuous variables (i.e. the basis of the local Hilbert space is a continuous basis).

In sharp contrast, for quantum lattice spin systems, the Hilbert space is naturally described by a discrete basis — $|S, M\rangle$ — where the quantum numbers are discrete (i.e. $0 \leq S \leq Ns$ and $M = -S, -S+1, ..., S-1, S$). This fact is a major problem in defining the path-integral for these systems and for doing it, we must build a new representation (perhaps overcomplete) that is labeled by continuous quantum numbers.

3.1. Quasi-Classical Spin States (Definition and Properties)

3.1.1. Schwinger Bosons Representation

References: [7,19]

We start by considering the simpler case of a single spin-s system, whose state is a ray in the $(2s+1)$-dimensional Hilbert Space — $\mathcal{H}_{site}$ — generated by the basis $\{|s, -s\rangle, |s, -s+1\rangle, ..., |s, s\rangle\}$. We can introduce a peculiar representation for the spin operators S^z and $S^{\pm}$ in terms of two kinds of bosonic operators[1], as first introduced by J. Schwinger [19].

$$S^+ = a^\dagger b \quad S^- = b^\dagger a \quad S^z = 1/2 \left\{ a^\dagger a - b^\dagger b \right\} \tag{3.1}$$

$$\left[a, a^\dagger\right] = \left[b, b^\dagger\right] = 1 \quad [a, a] = [b, b] = [a, b] = \left[a, b^\dagger\right] = 0$$

[1] In chapter 1, we have seen a representation in terms of only one kind of bosonic operators. In this case by using two, we obtain simpler expressions, at the expense of needing to specify extra constraints in order to specify the the spin multiplicity in question.

The verification that the above definitions do yield the correct algebra for the spin operators is done in [Appendix C.1]. In this language, the total spin operator S^2 can be written as [Appendix C.1]:

$$S^2 = 1/2\left(a^\dagger a + b^\dagger b\right)\left[1/2\left(a^\dagger a + b^\dagger b\right) + 1\right] \tag{3.2}$$

Finally, (3.1) and (3.2) allow us to interpret the number of a- and b-type bosons as follows:

$$s = 1/2\,(n_a + n_b)\,; \quad m = 1/2\,(n_a - n_b) \tag{3.3}$$

In order to fix the multiplicity of spin, we must restrict the Fock Space of the Schwinger bosons to the physical subspace, where $n_a + n_b = 2s$. In fact, by using the general properties of bosonic Fock-states, we can write any normalized state $|s,m\rangle$ as follows:

$$|s,m\rangle = |n_a = s+m, n_b = s-m\rangle = \frac{\left(a^\dagger\right)^{s+m}\left(b^\dagger\right)^{s-m}}{\sqrt{(s+m)!\,(s-m)!}}\,|0\rangle \tag{3.4}$$

3.1.2. Spin Coherent-States for a Single Spin

References: [7,12,13,17]

In this subsection, we wish to build a set of spin coherent-states, in complete analogy to the usual harmonic oscillator (see [10] for a full discussion of the harmonic oscillator coherent-state formalism). For that, it is important to emphasize that a quantum spin is not a 3-vector and the commutation relations (1.3) imply the following **Heisenberg Uncertainty Relation among the spin components** (derivation done in [Appendix C.2]):

$$\sqrt{\left\langle\left(S^x - \langle S^x\rangle\right)^2\right\rangle\left\langle\left(S^y - \langle S^y\rangle\right)^2\right\rangle} \geq 1/2\,|\langle S^z\rangle| \tag{3.5}$$

The relation (3.5) indicates that, even when the z-axis projection of the spin is known, there is a complete uncertainty in the value of the other two components (which cannot even be measured simultaneously). A good measure of this uncertainty is the variance of the x-component of the spin, given as — $\sigma_x^2(s,m) = \langle s,m|\left(S^x - \langle S^x\rangle\right)^2|s,m\rangle = \langle s,m|\left(S^x\right)^2|s,m\rangle$.[2] Using equation (3.5) and the property discussed in the footnote 2, we can write the following:

$$\sigma_x^2(s,m) = 1/2\left\langle\left(S^y\right)^2 + \left(S^y\right)^2\right\rangle = 1/2\left\langle S^2 - \left(S^z\right)^2\right\rangle = \frac{1}{2}s(s+1) - \frac{1}{2}m^2 \tag{3.6}$$

[2]Since the state $|s,m\rangle$ is invariant (up to a global phase) under rotations about the z-axis, we can write the variance of the spin component in a transverse direction that makes and angle θ with the x-axis, as:

$$\sigma_\theta^2(s,m) = \langle s,m|\left(S^\theta - \left\langle S^\theta\right\rangle\right)^2|s,m\rangle = \langle s,m|\left(\cos\theta S^x + \sin\theta S^y\right)^2|s,m\rangle =$$
$$= \langle s,m|\,U(\theta)^\dagger U(\theta)\left(S^x\right)^2 U(\theta)^\dagger U(\theta)\,|s,m\rangle = \sigma_x^2(s,m)$$

In particular, we have $\left\langle\left(S^x\right)^2\right\rangle = \left\langle\left(S^y\right)^2\right\rangle = 1/2\left\langle\left(S^y\right)^2 + \left(S^y\right)^2\right\rangle$.

This last result highlights that not all the states $|s,m\rangle$ yield the same perpendicular uncertainty. In fact, the ones that minimize it, are the extremal ones — $|s,\pm s\rangle$.

This situation is reminiscent from the study of the eigenstates of the quantum harmonic oscillator and the corresponding uncertainty between the position and linear-momentum. In that case, the eigenstate which minimized the product — $\langle\delta x\rangle\langle\delta p_x\rangle$ — was the ground-state[3]. As it is, this state has zero position and momentum average, but it can be used to create a minimum uncertainty state around any phase-point $(\overrightarrow{\mathbf{q}},\overrightarrow{\mathbf{p}})$, by acting on it with a displacement operator — $D(\alpha)$[4].

In our case, we wish to do something similar with the state $|s,s\rangle$ and generate a minimum uncertainty state, that is also an eigenstate of the spin component along an arbitrary axis. If that axis is represented by the unit vector $\hat{\Omega}$ (in spherical coordinates, it will be $\hat{\Omega}=(\cos\phi\sin\theta,\sin\phi\sin\theta,\cos\theta)$), then for orienting the z-axis with $\hat{\Omega}$, we must implement a rotation parametrized by the **Euler angles** (ϕ,θ,χ), as seen in the Figure 3.1. This is done by acting with the unitary operator defined in (3.7).[5]

$$U(\Omega)=U(\phi,\theta,\chi)=e^{-i\chi\widetilde{S}^z}e^{-i\theta\tilde{S}^y}e^{-i\phi S^z}=e^{-i\theta\tilde{S}^y}e^{-i\phi S^z}e^{-i\chi S^z}=e^{-i\phi S^z}e^{-i\theta S^y}e^{-i\chi S^z} \tag{3.7}$$

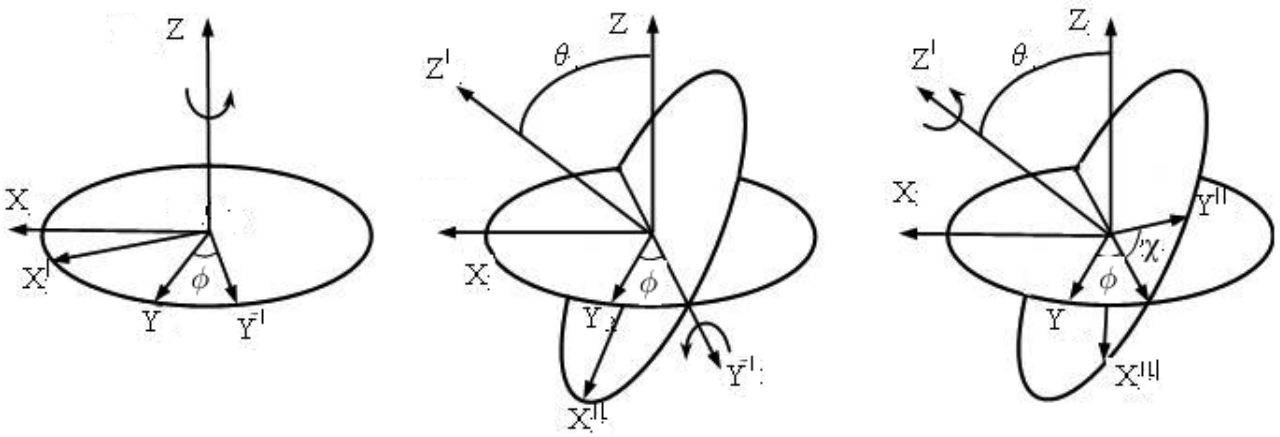


Figure 3.1.: Convention used for the Euler Angles — (ϕ,θ,χ) — used in the definition of the Spin Coherent-States. Refs. [11,39]

Therefore, the minimum uncertainty state pointing in the direction $\hat{\Omega}$ is just the one given by:[6]

$$\left|\hat{\Omega}^s\right\rangle=e^{-i\phi S^z}e^{-i\theta S^y}e^{-i\chi S^z}\left|s,s\right\rangle=e^{-is\chi}\left[e^{-i\phi S^z}e^{-i\theta S^y}\left|s,s\right\rangle\right] \tag{3.8}$$

The states $\left|\hat{\Omega}^s\right\rangle$ are called **Spin Coherent-States**. In (3.8), the choice of χ is irrelevant and we can

[3]Which is known to be a gaußian wavefunction.

[4]More precisely, the coherent state $|\alpha\rangle=D(\alpha)|0\rangle$ is a minimum uncertainty state, such that the real and imaginary parts of $\alpha\in\mathbb{C}$ are proportional to the average position and momentum, respectively.

[5]In (3.7), we assume the definitions $\widetilde{S}^y=e^{-i\phi S^z}S^y e^{i\phi S^z}$ and $\widetilde{S}^z=e^{-i\theta\tilde{S}^y}e^{-i\phi S^z}S^z e^{i\phi S^z}e^{i\theta\tilde{S}^y}$, which are just the spin components along the axis Y' and Z' (respectively), as seen in Figure 3.1

[6]It is worth noticing that:

$$\hat{\Omega}\cdot\overrightarrow{S}\left|\hat{\Omega}^s\right\rangle=U(\hat{\Omega})S^zU(\hat{\Omega})^\dagger U(\hat{\Omega})\left|s,m\right\rangle=sU(\hat{\Omega})\left|s,m\right\rangle=s\left|\hat{\Omega}^s\right\rangle$$

take the convention that $\chi = 0$, for all the states $\left|\hat{\Omega}^s\right\rangle$. Now, we use the results of [Appendix C.1] to write the rotated Schwinger operators, in terms of the original ones. This goes as follows:

$$\begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix} \underset{\mathcal{R}_{\phi,\theta,\chi}}{\longmapsto} \begin{pmatrix} \widetilde{a^\dagger} \\ b^\dagger \end{pmatrix} = e^{-i\sigma^z \frac{\phi}{2}} \cdot e^{-i\sigma^y \frac{\theta}{2}} \cdot \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix} = \begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix} \cdot \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix} \tag{3.9}$$

For $u(\theta,\phi) = e^{-i\phi/2}\cos\theta/2$, $v(\theta,\phi) = e^{i\phi/2}\sin\theta/2$ and $\widetilde{a}^\dagger/\widetilde{b}^\dagger$ being the Schwinger operators relative to the new quantization axis. From footnote 6, we know that $\left|\hat{\Omega}^s\right\rangle$ is a normalized $m = s$ eigenstate of the spin projection along $\hat{\Omega}$. This means that:

$$\left|\hat{\Omega}^s\right\rangle = \frac{\left(\widetilde{a}^\dagger\right)^{2s}}{\sqrt{(2s)!}} \left|0\right\rangle \tag{3.10}$$

By using (3.9), we are able to express (3.10) entirely in terms of the original Schwinger operators, yielding the result (3.11).

$$\begin{aligned} \left|\hat{\Omega}^s\right\rangle = \frac{\left(ua^\dagger + vb^\dagger\right)^{2s}}{\sqrt{(2s)!}} \left|0\right\rangle = \sqrt{(2s)!} \sum_{m=-s}^{+s} \frac{\left(ua^\dagger\right)^{s-m}\left(vb^\dagger\right)^{s+m}}{(s+m)!\,(s-m)!} \left|0\right\rangle = \\ = \sqrt{(2s)!} \sum_{m=-s}^{+s} \frac{u^{s-m}v^{s+m}}{\sqrt{(s+m)!\,(s-m)!}} \left|s,m\right\rangle \end{aligned} \tag{3.11}$$

As expected, the spin coherent-state — $\left|\hat{\Omega}^s\right\rangle$ — is a linear superposition of all the $|s,m\rangle$ states.

At last, we have a set of spin states which are labeled by a continuum of quantum numbers (namely the ϕ and θ coordinates of the vector $\hat{\Omega}$). Next, we must prove that these do form a basis for the local space $\mathcal{H}_{site}$ and derive the metric associated with them (i.e. the overlapping between any two spin coherent-states). These two results are carefully derived in [Appendix C.3] and we just write here the important results:

$$\left\langle \hat{\Omega}_2^s \mid \hat{\Omega}_1^s \right\rangle = \left[\frac{1 + \hat{\Omega}_1 \cdot \hat{\Omega}_2}{2}\right]^s e^{i\Psi(\hat{\Omega}_1,\hat{\Omega}_2)} \tag{3.12}$$

For a phase function defined as follows:

$$\Psi(\hat{\Omega}_1,\hat{\Omega}_2) \equiv 2s \arctan\left\{\tan\left(\frac{\phi_2 - \phi_1}{2}\right) \frac{\cos\left(\frac{\theta_1+\theta_2}{2}\right)}{\cos\left(\frac{\theta_1-\theta_2}{2}\right)}\right\}$$

And also:

$$\left(\frac{2s+1}{4\pi}\right) \int_{S^2} d\hat{\Omega} \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| = \left(\frac{2s+1}{4\pi}\right) \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \left|\theta,\phi\right\rangle \left\langle\theta,\phi\right| = \mathbb{I}^s \tag{3.13}$$

From the last two equations, we draw the following conclusions:

1. The set of spin coherent states is not orthogonal (though it is normalized). In fact, one sees from (3.12) that, only oppositely oriented states ($\hat{\Omega}_1 \cdot \hat{\Omega}_2 = -1$) are exactly orthogonal and also that the basis $\left|\hat{\Omega}^s\right\rangle$ becomes orthogonal in the classical limit $s \to +\infty$.[7]
2. Any state in $\mathcal{H}_{site}$ can be expressed as a linear superposition of non-orthogonal spin coherent-states. They form an over-complete basis of the Hilbert Space for a single spin.

Having a basis of states, we can use it to represent both vectors and operators. In the case of the spin coherent-states, it is clear that we can represent any ket $|\Psi\rangle \in \mathcal{H}_{site}$, as follows:

$$|\Psi\rangle = \left(\frac{2s+1}{4\pi}\right) \int_{S^2} d\hat{\Omega} \left|\hat{\Omega}^s\right\rangle \left\langle \hat{\Omega}^s \mid \Psi \right\rangle = \left(\frac{2s+1}{4\pi}\right) \int_{S^2} d\hat{\Omega}\ f_\Psi(\hat{\Omega}) \left|\hat{\Omega}^s\right\rangle \tag{3.14}$$

The function $f_\Psi(\hat{\Omega})$ is the wavefunction for the state $|\Psi\rangle$ in the $\hat{\Omega}$-sphere.

One may try to do the same for a linear operator $A \in End\,(\mathcal{H}_{site})$, but the situation is not as clear, due to the nonorthogonality of the basis $\left|\hat{\Omega}^s\right\rangle$. To see why, let us take the representation given in (3.15):

$$A = \left(\frac{2s+1}{4\pi}\right)^2 \int\int_{S^2\times S^2} d\hat{\Omega}_1 d\hat{\Omega}_2\ a(\hat{\Omega}_1, \hat{\Omega}_2) \left|\hat{\Omega}_1^s\right\rangle \left\langle \hat{\Omega}_2^s\right| \tag{3.15}$$

Now, we may ask what is the form of the representative $a(\hat{\Omega}_1, \hat{\Omega}_2)$. If the basis were orthogonal and not overcomplete, one would prove immediately that $a(\hat{\Omega}_1, \hat{\Omega}_2) = \left\langle \hat{\Omega}_1^s\right| A \left|\hat{\Omega}_2^s\right\rangle$. But in this case, we get a different result:

$$\left\langle \hat{\Omega}_1^s\right| A \left|\hat{\Omega}_2^s\right\rangle = \left(\frac{2s+1}{4\pi}\right)^2 \int\int_{S^2\times S^2} d\Omega d\overline{\Omega}\ a(\Omega, \overline{\Omega}) \left\langle \Omega_1^s \mid \Omega^s\right\rangle \left\langle \overline{\Omega}^s \mid \Omega_2^s\right\rangle \tag{3.16}$$

And, since — $\left\langle \hat{\Omega}_1^s \mid \hat{\Omega}_2^s\right\rangle \neq \delta^{(2)}(\hat{\Omega}_1 - \hat{\Omega}_2)$ — the function $a(\hat{\Omega}_1, \hat{\Omega}_2)$ is not necessarily given by the matrix elements of A. This odd situation is lengthly discussed in Ref. [14], and it demonstrates a freedom in choosing the representative of an operator due to the excess of basis elements used in describing it.[8] In particular, it was proven by J. Kutzner in Refs. [15,16], that **any operator $A \in End\,(\mathcal{H}_{site})$ can be given a diagonal representation** in terms of spin coherent-states, as follows:

$$A = \frac{2s+1}{4\pi} \int_{S^2} d\Omega\ Tr\left[A \cdot \Delta_s(\hat{\Omega})\right] \left|\hat{\Omega}^s\right\rangle \left\langle \hat{\Omega}^s\right| \tag{3.17}$$

Where the trace is the usual — $\sum_{m=-s}^{s} \langle s, m|\, A \cdot \Delta_s(\hat{\Omega})\, |s, m\rangle$ — and the mapping operator $\Delta_s(\hat{\Omega})$ is defined as:[9]

[7] This is because $-1 \leq \hat{\Omega}_1 \cdot \hat{\Omega}_2 \leq 1$, since they are unit vectors. Note also that this result is nothing but another evidence for the irrelevance of the commutator between the spin components, in the large s limit.

[8] Note that $a(\Omega_1, \Omega_2) = \langle \Omega_1^s|\, A\, |\Omega_2^s\rangle$ is also a possible representation for the operator A. To prove that, one must only use the resolution of identity given in (3.1.15) and thus write $A = \left(\frac{2s+1}{4\pi}\right)^2 \int\int_{S^2\times S^2} d\Omega d\Omega'\, |\Omega_1^s\rangle \langle \Omega_1^s|\, A\, |\Omega_2^s\rangle \langle \Omega_2^s|$. But, since the basis is overcomplete, this definition is not unique.

[9] It is useful to note that the definition of the binomial coefficients is extended as: 1) $\begin{pmatrix} n \\ k \end{pmatrix} = 0$, if $n, k \geq 0$ and $n < k$; 2) $\begin{pmatrix} -n \\ k \end{pmatrix} = (-n)(-n-1)...(-n-k+1)$, if $n, k > 0$.

$$\Delta_s(z) = \frac{(-1)^{2s}}{(2s+1)!} \sum_{m_1,m_2=-s}^{s} |s,m_1\rangle \langle s,m_2| \sqrt{\frac{(s-m_1)!(s+m_1)!}{(s-m_2)!(s+m_2)!}} (z*)^{m_1-m_2} \times \tag{3.18}$$
$$\times \sum_{k=0}^{s+m_1} \sum_{r=0}^{s-m_1} (-1)^{k+r} \begin{pmatrix} s+m_2 \\ s+m_1-k \end{pmatrix} \begin{pmatrix} s-m_2 \\ s-m_1-r \end{pmatrix} \frac{(2s+1+k+r)!}{r!k!} \frac{|z|^{2r}}{(1+|z|^2)^{k+r}}$$

In (3.18), the variable z **is the stereographic coordinate** associated to the vector $\hat{\Omega}$ — defined as $z = e^{i\phi} \tan\theta/2$. In particular, by applying (3.17) to the components of the spin operator, we get the following important results:

$$S^x = \frac{(s+1)(2s+1)}{4\pi} \int_{S^2} d\Omega \sin\theta\cos\phi \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{3.19}$$

$$S^y = \frac{(s+1)(2s+1)}{4\pi} \int_{S^2} d\Omega \sin\theta\sin\phi \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{3.20}$$

$$S^z = \frac{(s+1)(2s+1)}{4\pi} \int_{S^2} d\Omega \cos\theta \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{3.21}$$

This can be condensed in the beautiful expression (3.22), using the vector notation — $\overrightarrow{S} = (S^x, S^y, S^z)$:

$$\overrightarrow{S} = \frac{(s+1)(2s+1)}{4\pi} \int_{S^2} d\Omega \overrightarrow{\Omega} \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{3.22}$$

The proof of Kutzner's Theorem, as well as the derivation of the expressions (3.19-22) are done in [Appendix C.4]. Finally, we also remark that the average of the spin components can be calculated in any state $\left|\hat{\Omega}^s\right\rangle$, using the last results. The final results are the following (results derived in [Appendix C.4]):

$$\left\langle\hat{\Omega}^s\right| S^x \left|\hat{\Omega}^s\right\rangle = s\sin\theta\cos\phi; \quad \left\langle\hat{\Omega}^s\right| S^y \left|\hat{\Omega}^s\right\rangle = s\sin\theta\cos\phi; \quad \left\langle\hat{\Omega}^s\right| S^z \left|\hat{\Omega}^s\right\rangle = s\cos\theta \tag{3.23}$$

Or, in vector notation:

$$\left\langle\hat{\Omega}^s\right| \overrightarrow{S} \left|\hat{\Omega}^s\right\rangle = s\overrightarrow{\Omega} \tag{3.24}$$

The result (3.22) will be useful for the last part of Chapter 4, while (3.24) will be essential for deriving the path-integral formulation of the Heisenberg Model.

3.1.3. Spin Coherent-States for a System of Many Spins

Up until now, we defined and studied the properties of the coherent-states associated to a single spin-s. But ultimately, we wish to treat the problem of a macroscopic system of many interacting spins in a

lattice. Fortunately, all of the above results can be trivially generalized to the Hilbert space of the full system of N spins — $\mathscr{H} = \mathcal{H}_{site}^{\otimes N}$. All we need to do, is rewrite the results in the proper way.

Starting from the the coherent-states for each localized spin, we define the manybody spin coherent-states $|\Omega\rangle$, as a tensor product of on-site coherent-states:

$$|\Omega\rangle = \otimes_{i\in\mathcal{L}} \left|\hat{\Omega}_i^s\right\rangle \tag{3.25}$$

Each state is labeled by a list of local spherical coordinates, i.e. $\Omega = \left\{\hat{\Omega}_i\right\}_{i\in\mathcal{L}}$[10]. The overlap function for these states can be easily computed, using the result (3.12):

$$\begin{aligned}\langle\Omega_2 \mid \Omega_1\rangle = \prod_{i\in\mathcal{L}} \left\langle \hat{\Omega}_{2i}^s \mid \hat{\Omega}_{1i}^s \right\rangle = \prod_{i\in\mathcal{L}} \left[\frac{1+\hat{\Omega}_{1i}\cdot\hat{\Omega}_{2i}}{2}\right]^s \times \\ \times \exp\left[2si \arctan\left\{\tan\left(\frac{\phi_{2i}-\phi_{1i}}{2}\right)\frac{\cos\left(\frac{\theta_{1i}+\theta_{2i}}{2}\right)}{\cos\left(\frac{\theta_{1i}-\theta_{2i}}{2}\right)}\right\}\right] = \prod_{i\in\mathcal{L}}\left\{\left[\frac{1+\hat{\Omega}_{1i}\cdot\hat{\Omega}_{2i}}{2}\right]^s\right\} e^{i\sum_i \Psi(\hat{\Omega}_{1i},\hat{\Omega}_{2i})}\end{aligned} \tag{3.26}$$

The definition of the phase function — Ψ — is the same as in (3.12). On the other hand, the identity operator in $\mathscr{H}$ is just given by:

$$\begin{aligned}\mathbb{I} = \otimes_{i\in\mathcal{L}}\mathbb{I}_i = \otimes_{i\in\mathcal{L}}\left\{\left(\frac{2s+1}{4\pi}\right)\int_{S^2} d\hat{\Omega}_i \left|\hat{\Omega}_i^s\right\rangle\left\langle\hat{\Omega}_i^s\right|\right\} = \\ = \prod_{i\in\mathcal{L}}\left\{\left(\frac{2s+1}{4\pi}\right)\int_{S^2} d\hat{\Omega}_i\right\} \otimes_{i\in\mathcal{L}} \left|\hat{\Omega}_i^s\right\rangle\left\langle\hat{\Omega}_i^s\right| = \left(\frac{2s+1}{4\pi}\right)^N \int d\Omega\, |\Omega\rangle\langle\Omega|\end{aligned} \tag{3.27}$$

Finally, we generalize the representation of the local spin operators $\overrightarrow{S}_i$[11]. After using (3.27) and (3.22), we arrive at the following result:

$$\overrightarrow{\mathbf{S}}_i = \left(\frac{2s+1}{4\pi}\right)^N (s+1)\int d\Omega \overrightarrow{\Omega_i}\, |\Omega\rangle\langle\Omega| \tag{3.28}$$

$$\langle\Omega|\,\overrightarrow{\mathbf{S}}_i\,|\Omega\rangle = s\hat{\Omega}_i \quad ; \quad \langle\Omega|\,\overrightarrow{\mathbf{S}}_i\cdot\overrightarrow{\mathbf{S}}_j\,|\Omega\rangle = s^2\hat{\Omega}_i\cdot\hat{\Omega}_j \tag{3.29}$$

We are now in possession of all the needed results on Spin Coherent-States to carry on with our reformulation of the Heisenberg Model as a path-integral. This will be the subject of the next section.

[10] Meaning that the parameter space for the many-spins coherent states is a direct product of N $\hat{\Omega}$-spheres.

[11] We point out that the natural extension of these operators to the entire Hilbert space is given by $[\otimes_{j\neq i}\mathbb{I}]\otimes\overrightarrow{S_i}$

3.2. Path-Integral Formulation for Lattice Spin Hamiltonians

3.2.1. The Generating Functional Method

References: [7,22]

When we are given a physical model, the main aim will always be the calculation of averages and correlations between operators in that system. In our case, it is interesting to calculate averages of spin operators and spin-spin correlation functions, between different sites and possibly at different times.

In thermodynamical equilibrium, the state of the system at a temperature — $T = \frac{1}{k_B \beta}$ — is given by the density operator — $\rho = e^{-\beta H_0}$ (where H_0 is the Hamiltonian operator). This density operator reflects only the thermal distribution among the states available for the system. But besides that, our quantum system also has a non-trivial unitary time-evolution, generated by the Hamiltonian. I.e.:

$$|\Psi(t)\rangle = U(t,0)\,|\Psi(0)\rangle \tag{3.30}$$

The operator $U(t,J)$ represents a time-evolution generated by — $H[J(t)] = H_0 + \sum_{i,\alpha} J_i^\alpha(t) S_i^\alpha(t)$ — which includes a coupling of the relevant operators with external local fields $J_i^\alpha(t)$ (i represents the lattice site and $\alpha = x, y, z$)[12] This operator can be written formally as a time-ordered exponential, as is well known from Quantum Mechanics:

$$U(t,J) = \mathcal{T}_t \left\{ \exp\left[-i \int_0^t dt' H[J] \right] \right\} \Rightarrow U(t,0) = e^{-iH_0 t} \tag{3.31}$$

The last equality in (3.31) comes from the fact that the free Hamiltonian is time-independent.

The average of a spin operator (in the Heisenberg picture) and the correlation function between spins can be given as follows:

$$\langle S_i^\alpha(t) \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} e^{-iH_0 t} S_i^\alpha(0) e^{iH_0 t} \right\} \tag{3.32}$$

$$C_{ij}^{\alpha\beta}(t',t) = \left\langle \mathcal{T}_t \left[S_i^\alpha(t') S_j^\beta(t) \right] \right\rangle = \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} \mathcal{T}_t \left[e^{-iH_0 t'} S_i^\alpha(0) e^{iH_0(t'-t)} S_j^\beta(0) e^{iH_0 t} \right] \right\} \tag{3.33}$$

Where the partition function Z is defined as usual, by — $Z = \mathrm{Tr}\left[e^{-\beta H_0} \right]$.

Equations (3.32) and (3.33) express the quantities of interest and are directly related to the predictions of any spin model. In order to calculate them, we can resort to a clever trick from Quantum Field Theory, called the **Method of the Generating Functional**. The first step one must perform is to Wick-rotate the expressions (3.32) and (3.33), by setting $t \to -i\tau$:

$$\langle S_i^\alpha(\tau) \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} e^{-H_0 \tau} S_i^\alpha(0) e^{H_0 \tau} \right\} \tag{3.34}$$

[12] Any probing of the properties of the system will always include weak couplings with external classical fields.

$$C_{ij}^{\alpha\beta}(\tau',\tau) = \left\langle \mathcal{T}_\tau \left[S_i^\alpha(\tau') S_j^\beta(\tau) \right] \right\rangle = \frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta H_0} \mathcal{T}_\tau \left[e^{-H_0 \tau'} S_i^\alpha(0) e^{H_0(\tau'-\tau)} S_j^\beta(0) e^{iH\tau} \right] \right\} \tag{3.35}$$

Then, we define the Generating Functional for the model, as follows:[13]

$$\begin{aligned} Z[J(\tau)] &= \mathrm{Tr} \left\{ T_\tau \left[\exp \left\{ - \int_0^\beta d\tau H[J(\tau)] \right\} \right] \right\} = \\ &= \mathrm{Tr} \left\{ T_\tau \left[\exp \left\{ - \int_0^\beta d\tau \left(H_0 + \sum_{i,\alpha} J_i^\alpha(\tau) S_i^\alpha(\tau) \right) \right\} \right] \right\} \end{aligned} \tag{3.36}$$

It is clear that (3.34) and (3.35) can be written as functional derivatives of (3.36) with respect to the source functions — $J_i^\alpha(\tau)$ — as given in the next two equations. A review of these facts is given in [Appendix C.5].

$$\langle S_i^\alpha(\tau) \rangle = \frac{1}{Z[0]} \frac{\delta Z[J(\tau)]}{\delta J_i^\alpha(\tau)} \mid_{J=0} \tag{3.37}$$

$$C_{ij}^{\alpha\beta}(\tau',\tau) = \frac{1}{Z[0]} \frac{\delta Z[J(\tau)]}{\delta J_i^\alpha(\tau') \delta J_j^\beta(\tau)} \mid_{J=0} \tag{3.38}$$

3.2.2. Building the Spin Path-Integral

References: [6,7,20,21]

It is evident that the important thing to calculate is the Generating Functional — $Z[J(\tau)]$. In this section, we will see that it is possible to re-express (3.36) as a path-integral written in the space of the coherent-state parameters $\hat{\Omega}$. To do that, we proceed in a fashion similar to the way path-integrals are built in ordinary quantum mechanics and field theory [20,21,22].

We start by breaking up the time interval — $[0, \beta]$ — into $k+1$ infinitesimal slices of width ϵ. That allows us to write the following:

$$Z[J(\tau)] = \int d\Omega(0) \, \langle \Omega(\beta) | \, e^{-H[J(\beta-\epsilon)]\epsilon} ... e^{-H[J(\epsilon)]\epsilon} e^{-H[J(0)]\epsilon} \, | \Omega(0) \rangle \tag{3.39}$$

The time-ordering symbol was removed, since the equation — $\mathcal{T}_\tau(\exp\left\{ - \int_t^{t+\epsilon} d\tau H[J(\tau)] \right\}) = e^{-H[J(t)]\epsilon}$ — is true to first order in the small ϵ. Furthermore, if (3.39) is to represent a trace, one must impose the usual constraint of periodicity in the imaginary time, i.e. — $\Omega(\beta) = \Omega(0)$.[14]

Now, we can place in between the exponential factors, the resolutions of identity derived in (3.27). This way, we obtain the following discretized version of the functional:

[13] Note that $Z[0]$ is just the good old canonical partition function, used in (3.32) and (3.33).

[14] It is not obvious that the trace in the definition of the Generating Functional can be written in the basis of spin coherent-states, since it is not an orthonormal basis of the Hilbert Space. However in the [Appendix C.6] we prove that the trace calculated in the standard basis or in the coherent-states do yield the same value, justifying the expression (3.39).

$$Z_\epsilon[J(\tau)] = \int d\Omega(0) \left[\prod_{n=1}^{k} \left(\frac{2s+1}{4\pi} \right)^N \int d\Omega_n \right] \langle \Omega(0)| \, e^{-H[J(\beta-\epsilon)]\epsilon} \, |\Omega_k\rangle \, \langle \Omega_k| \, ... \, |\Omega_1\rangle \, \langle \Omega_1| \, e^{-H[J(0)]\epsilon} \, |\Omega(0)\rangle \tag{3.40}$$

From (3.40), it is clear that we must deal with a bunch of terms like the one that follows:

$$\begin{aligned} \langle \Omega(\tau+\epsilon)| \, e^{-H[J(\tau)]\epsilon} \, |\Omega(\tau)\rangle &= \langle \Omega(\tau+\epsilon)| \, 1 - H[J(\tau)]\epsilon + ... \, |\Omega(\tau)\rangle = \\ &= \langle \Omega(\tau+\epsilon) \mid \Omega(\tau)\rangle \left\{ 1 - \frac{\langle \Omega(\tau+\epsilon)| \, H[J(\tau)] \, |\Omega(\tau)\rangle}{\langle \Omega(\tau+\epsilon) \mid \Omega(\tau)\rangle} \epsilon + ... \right\} = \qquad (3.41) \\ &= \langle \Omega(\tau+\epsilon) \mid \Omega(\tau)\rangle \, e^{-\mathcal{H}_{cl}[J(\tau)]\epsilon} \qquad (3.42) \end{aligned}$$

The classical Hamiltonian $\mathcal{H}_{cl}$ being defined in (3.41), as:

$$\mathcal{H}_{cl}[J(\tau)] = \frac{\langle \Omega(\tau+\epsilon)| \, H[J(\tau)] \, |\Omega(\tau)\rangle}{\langle \Omega(\tau+\epsilon) \mid \Omega(\tau)\rangle} = \langle \Omega(\tau)| \, H[J(\tau)] \, |\Omega(\tau)\rangle \, \{1 + \mathcal{O}(\epsilon)\}$$

For the last expansion, we used the following fact:

$$|\Omega(\tau+\epsilon)\rangle = |\Omega(\tau)\rangle + \epsilon \frac{d}{d\tau'} \left| \Omega(\tau') \right\rangle |_{\tau'=\tau} + \mathcal{O}(\epsilon^2) \tag{3.43}$$

Specializing for the Heisenberg Model, we get:[15]

$$\begin{aligned} \mathcal{H}_{cl}[\overrightarrow{B}(\tau)] &= J \, \langle \Omega(\tau)| \sum_{\langle i,j\rangle \in \mathscr{L}} \overrightarrow{S}_i \cdot \overrightarrow{S}_j + \sum_{i \in \mathscr{L}} \overrightarrow{B}(\tau, x_i) \cdot \overrightarrow{S}_i \, |\Omega(\tau)\rangle + \mathcal{O}(\epsilon) = \\ &= Js^2 \sum_{\langle i,j\rangle \in \mathscr{L}} \hat{\Omega}_i(\tau) \cdot \hat{\Omega}_j(\tau) + s \sum_{i \in \mathscr{L}} \overrightarrow{B}(\tau, x_i) \cdot \hat{\Omega}_i(\tau) + \mathcal{O}(\epsilon) \end{aligned} \tag{3.44}$$

Where we used the result (3.29). Using (3.43), we can also expand the overlap function in (3.42) as a power series in ϵ. It yields the following expression:

$$\left\langle \overrightarrow{\Omega}(\tau+\epsilon) \mid \overrightarrow{\Omega}(\tau) \right\rangle = 1 + \epsilon \frac{d}{d\tau'} \left\langle \overrightarrow{\Omega}(\tau') \mid \overrightarrow{\Omega}(\tau) \right\rangle |_{\tau'=\tau} + \mathcal{O}(\epsilon^2) \tag{3.45}$$

[15] Note that in this particular case, the field coupled to the local spin operators - $\overrightarrow{B}(\tau, x_i)$ - is an external magnetic field, multiplied by the gyromagnetic ratio.

The first order term can be obtained by directly expanding (3.27), which yields:

$$\langle \Omega(\tau+\epsilon) \mid \Omega(\tau) \rangle = \prod_{i \in \mathcal{L}} \left[\frac{1 + \left| \hat{\Omega}_i(\tau) \right|^2 + \epsilon \left[\frac{d}{d\tau} \hat{\Omega}_i(\tau) \right] \cdot \hat{\Omega}_i(\tau) + ...}{2} \right]^s \times$$
$$\times \exp \left[2si \arctan \left\{ \tan \left(\epsilon \frac{\dot{\phi}_i(\tau)}{2} + ... \right) \frac{\cos \left(\theta_i(\tau) + \frac{\epsilon}{2} \dot{\theta}_i(\tau) + ... \right)}{\cos \left(-\frac{\epsilon}{2} \dot{\theta}_i(\tau) + ... \right)} \right\} \right] \tag{3.46}$$

Noting that $\frac{d}{d\tau} \hat{\Omega}_i(\tau)$ is orthogonal to $\hat{\Omega}_i(\tau)$ (since the length of the vector $\hat{\Omega}$ is kept always equal to 1), we have:

$$\langle \Omega(\tau+\epsilon) \mid \Omega(\tau) \rangle = \prod_{i \in \mathcal{L}} \exp \left[2si \arctan \left\{ \epsilon \frac{\dot{\phi}_i(\tau)}{2} \cos\left(\theta_i(\tau)\right) + ... \right\} \right] =$$
$$= \prod_{i \in \mathcal{L}} \left\{ 1 + is\epsilon \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) + ... \right\} = 1 + is\epsilon \sum_{i \in \mathscr{L}} \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) + \mathcal{O}(\epsilon^2) \tag{3.47}$$

Hence, applying the expressions (3.44) and (3.47) to the infinitesimal propagator given in (3.42), we get:

$$\left\langle \overrightarrow{\Omega}(\tau+\epsilon) \right| e^{-H[J(\tau)]\epsilon} \left| \overrightarrow{\Omega}(\tau) \right\rangle = \left[1 + is\epsilon \sum_{i \in \mathscr{L}} \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) + \mathcal{O}(\epsilon^2) \right] \times$$
$$\times \left[1 - \epsilon J s^2 \sum_{\langle i,j \rangle \in \mathscr{L}} \overrightarrow{\Omega}_i(\tau) \cdot \overrightarrow{\Omega}_j(\tau) - \epsilon s \sum_{i \in \mathscr{L}} \overrightarrow{B}(\tau, x_i) \cdot \overrightarrow{\Omega}_i(\tau) + \mathcal{O}(\epsilon^2) \right] =$$
$$= 1 + \left\{ is \sum_{i \in \mathscr{L}} \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) - Js^2 \sum_{\langle i,j \rangle \in \mathscr{L}} \overrightarrow{\Omega}_i(\tau) \cdot \overrightarrow{\Omega}_j(\tau) - s \sum_{i \in \mathscr{L}} \overrightarrow{B}(\tau, x_i) \cdot \overrightarrow{\Omega}_i(\tau) \right\} \epsilon + \mathcal{O}(\epsilon^2) =$$
$$= \exp \left[\left\{ is \sum_{i \in \mathscr{L}} \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) - Js^2 \sum_{\langle i,j \rangle \in \mathscr{L}} \overrightarrow{\Omega}_i(\tau) \cdot \overrightarrow{\Omega}_j(\tau) - s \sum_{i \in \mathscr{L}} \overrightarrow{B}(\tau, x_i) \cdot \overrightarrow{\Omega}_i(\tau) \right\} \epsilon \right] \tag{3.48}$$

Finally, we must plug (3.48) into the discretized Generating Functional (3.40), yielding:

$$Z_\epsilon[\overrightarrow{B}(\tau)] = \int d\Omega(0) \left[\prod_{n=1}^{k} \left(\frac{2s+1}{4\pi} \right)^N \int d\Omega_n \right] \exp \left[\sum_{n=0}^{k} \left\{ is \sum_{i \in \mathscr{L}} \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) - \mathcal{H}_{Heis}[\overrightarrow{B}(\tau)] \right\} \epsilon \right] =$$
$$= \frac{1}{A} \left[\prod_{n=1}^{k} \int d\Omega_n \right] \exp \left[\sum_{n=0}^{k} \left\{ is \sum_{i \in \mathscr{L}} \dot{\phi}_i(\tau) \cos\left(\theta_i(\tau)\right) - \mathcal{H}_{Heis}[\overrightarrow{B}(\tau)] \right\} \epsilon \right] \tag{3.49}$$

By taking the formal continuum-limit in the time variable[16], we get the final path-integral formulation for the Heisenberg spin model:

$$Z[\overrightarrow{B}(\tau)] = \oint \mathscr{D}\overrightarrow{\Omega}(\tau) \exp\left[-s\int_0^\beta d\tau \left\{-i\sum_{i\in\mathscr{L}} \dot{\phi}_i(\tau)\cos\left(\theta_i(\tau)\right) + \right.\right.$$
$$\left.\left. + Js \sum_{\langle i,j\rangle\in\mathscr{L}} \overrightarrow{\Omega}_i(\tau)\cdot\overrightarrow{\Omega}_j(\tau) + + \sum_{i\in\mathscr{L}} \overrightarrow{B}(\tau,x_i)\cdot\overrightarrow{\Omega}_i(\tau)\right\}\right] \tag{3.50}$$

And the integral sign is cyclic — $\oint$ — because we must only sum over configurations that obey the constraint — $\Omega(0) = \Omega(\beta)$.

The path-integral description given in (3.50) takes the form one would naively expect. The only exception being the first term in the action, which is imaginary, even though we are already working in imaginary time. This new term — (3.51) — is called a **Berry phase** and, as will be seen, it has a topological origin.

$$\omega[\hat{\Omega}_i] = -\int_0^\beta d\tau \frac{d\phi_i(\tau)}{d\tau}\cos\left(\theta_i(\tau)\right) \tag{3.51}$$

As pointed out in Ref. [7], these terms can be written using a $U(1)$-gauge field defined in the space of the parameters Ω. The corresponding vector potential is just:

$$\overrightarrow{A}[\hat{\Omega}_i] = -\frac{\cos\theta_i}{\sin\theta_i}\hat{\phi}_i \tag{3.52}$$

Which yields (after noticing that — $\dot{\hat{\Omega}}_i(\tau) = \dot{\phi}_i \sin\theta_i\hat{\phi}_i + \dot{\theta}_i\hat{\theta}_i$):

$$\omega[\hat{\Omega}_i] = \int_0^\beta d\tau \overrightarrow{A}[\hat{\Omega}_i(\tau)]\cdot\dot{\hat{\Omega}}_i(\tau) \tag{3.53}$$

It is worth noting that (3.52) generates a monopolar 'magnetic-field' in the space of parameters, as can be seen from a direct calculation:

$$\overrightarrow{B}(\hat{\Omega}_i) = \nabla\times\overrightarrow{A}(\hat{\Omega}_i) = \frac{1}{r}\hat{\Omega} \tag{3.54}$$

The Berry phase is the flux of $\overrightarrow{B}(\hat{\Omega}_i)$ across the $\hat{\Omega}$-sphere. With these last definitions, the final form of the generating functional for the spin lattice system will be:

[16] As usual the constant A, although irrelevant for calculating averages, is needed to regularize the continuum limit. See [22] for a general discussion.

$$Z[\overrightarrow{B}(\tau)] = \oint \mathscr{D}\Omega(\tau) \exp\left[-is\sum_{i\in\mathscr{L}}\omega[\hat{\Omega}_i(\tau)] - s\int_0^\beta d\tau\left\{Js\sum_{\langle i,j\rangle\in\mathscr{L}}\hat{\Omega}_i(\tau)\cdot\hat{\Omega}_j(\tau) + \sum_{i\in\mathscr{L}}\overrightarrow{B}(\tau,x_i)\cdot\hat{\Omega}_i(\tau)\right\}\right] \tag{3.55}$$

3.3. The Haldane Mapping to the $\mathcal{O}(3)$ Non-Linear Sigma Model

References: [6,7,23,24]

The path-integral formulation of the Heisenberg model — (3.55) — is entirely equivalent to the one that uses the Hamiltonian operator. However, it offers the opportunity of describing the physics of the lattice model by means of a **Coarse-Grained Continuous Néel Field** - $\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}})$ - which will be described by an effective action. Such a description was first obtained by F. D. M. Haldane (for the Heisenberg AFM model) on 1983 [23,24], and was mainly based on expanding the Heisenberg Hamiltonian, in a way that does not break the rotational symmetry (which was the main drawback of 'Spin-Wave Theory').

To obtain the effective continuum theory, we start by promoting the lattice variables $\hat{\Omega}_i(\tau)$ to a continuous function of the spacial variable $\overrightarrow{\mathbf{x}}$ — $\overrightarrow{\mathbf{\Omega}}(\tau,\overrightarrow{\mathbf{x}})$. Using this new **Spin Field**, the Euclidean action for the model (in the absence of an external field) is written as:

$$S[\hat{\Omega}(\tau,\overrightarrow{\mathbf{x}}_i)] = is\sum_{i\in\mathscr{L}}\omega[\hat{\Omega}(\tau,\overrightarrow{\mathbf{x}}_i)] + Js^2\int_0^\beta d\tau\left\{\sum_{\langle i,j\rangle\in\mathscr{L}}\hat{\Omega}(\tau,\overrightarrow{\mathbf{x}}_i)\cdot\hat{\Omega}(\tau,\overrightarrow{\mathbf{x}}_j)\right\} \tag{3.56}$$

To proceed, we must take the following ideas into account:

1. Even if the there is no long-range Néel order, the correlations at small distances will still be of the Néel type;
2. In the path-integral, we will disregard of all the field configurations that vary appreciably over distances of a few lattice spacings[17]
3. The contributions to the spin field can be separated into a **Main Néel Field** — $\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})$ — and a **Canting Field** — $\overrightarrow{\mathbf{K}}(\tau,\overrightarrow{\mathbf{x}})$ — that represent the perpendicular fluctuations about the main field (i.e. — $\overrightarrow{\mathbf{K}}(\tau,\overrightarrow{\mathbf{x}})\cdot\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}}) = 0$)[18]. In terms of these fields, $\overrightarrow{\mathbf{\Omega}}(\tau,\overrightarrow{\mathbf{x}})$ can be written as follows:

[17] Here, we will assume that the lattice is a d-dimensional hypercubic, with lattice parameter a.

[18] A comment is in order, regarding the number of degrees of freedom. In fact, by doing this description we are replacing the original $2N$ degrees of freedom, by the double of them. This is not justifiable in general, but in this case can be done, because we will ignore all the Fourier components of $\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})$, except the hydrodynamic ones — i.e. $\left|\overrightarrow{\mathbf{k}}\right| \leq \frac{\pi}{\Lambda}$, where $a \ll \Lambda \ll Na$ is a small-distance cut-off.

$$\overrightarrow{\mathbf{\Omega}}(\tau, \overrightarrow{\mathbf{x}}_j) = \eta_j \overrightarrow{\mathbf{n}}(\tau, \overrightarrow{\mathbf{x}}_j)\sqrt{1 - \left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right|^2} + \frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s} \tag{3.57}$$

Where $\eta_i = e^{i\overrightarrow{\mathbf{x}}_j \cdot \overrightarrow{\pi}/a}$, a is the lattice parameter and $\overrightarrow{\pi} = (\pi, ..., \pi)$.

We also need to guarantee that the normalization constraint — $\left|\overrightarrow{\mathbf{\Omega}}(\tau, \overrightarrow{\mathbf{x}}_j)\right|^2 = 1$ — still holds in (3.57), i.e. :

$$\begin{aligned}\overrightarrow{\mathbf{\Omega}}(\tau, \overrightarrow{\mathbf{x}}_j) \cdot \overrightarrow{\mathbf{\Omega}}(\tau, \overrightarrow{\mathbf{x}}_j) = \left|\overrightarrow{\mathbf{n}}(\tau, \overrightarrow{\mathbf{x}}_j)\right|^2 \left[1 - \left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right|^2\right] + \left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right|^2 + \\ + 2\eta_j \overrightarrow{\mathbf{n}}(\tau, \overrightarrow{\mathbf{x}}_j) \cdot \overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)\sqrt{1 - \left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right|^2} = 1\end{aligned} \tag{3.58}$$

Which implies that the main Néel field must be also unimodular:

$$\left|\overrightarrow{\mathbf{n}}(\tau, \overrightarrow{\mathbf{x}}_j)\right|^2 = 1 \tag{3.59}$$

We will assume, in further calculations, that $\left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right| \ll 1$ and keep only terms till first-order in this quantity. Then, the spin field can be approximated as:

$$\overrightarrow{\mathbf{\Omega}}(\tau, \overrightarrow{\mathbf{x}}_j) \approx \eta_j \overrightarrow{\mathbf{n}}(\tau, \overrightarrow{\mathbf{x}}_j) + \frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s} - \frac{1}{2}\eta_j \overrightarrow{\mathbf{n}}(\tau, \overrightarrow{\mathbf{x}}_j)\left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right|^2 + \mathcal{O}\left(\left|\frac{\overrightarrow{\mathbf{K}}(\tau, \overrightarrow{\mathbf{x}}_j)}{s}\right|^4\right) \tag{3.60}$$

3.3.1. Continuum Approximation for the Spin Hamiltonian

To obtain an effective QFT action for the Néel field, we start by using the expansion (3.60) to express the classical Hamiltonian — $\mathcal{H}_{cl} = s^2 \sum_{i,j} J_{ij} \overrightarrow{\mathbf{\Omega}}_i \cdot \overrightarrow{\mathbf{\Omega}}_j$ — as follows[19]:

$$\begin{aligned}\overrightarrow{\mathbf{\Omega}}_i \cdot \overrightarrow{\mathbf{\Omega}}_j \approx \eta_i\eta_j \overrightarrow{\mathbf{n}}_i \cdot \overrightarrow{\mathbf{n}}_j + \frac{1}{s}\left(\eta_i \overrightarrow{\mathbf{n}}_i \cdot \overrightarrow{\mathbf{K}}_j + \eta_j \overrightarrow{\mathbf{n}}_j \cdot \overrightarrow{\mathbf{K}}_i\right) + \\ + \frac{1}{s^2}\left[\overrightarrow{\mathbf{K}}_i \cdot \overrightarrow{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j \overrightarrow{\mathbf{n}}_i \cdot \overrightarrow{\mathbf{n}}_j \left(\left|\overrightarrow{\mathbf{K}}_i\right|^2 + \left|\overrightarrow{\mathbf{K}}_j\right|^2\right)\right] + ...\end{aligned} \tag{3.61}$$

If we use the fact that $\left|\overrightarrow{\mathbf{n}}_i\right|^2 = \left|\overrightarrow{\mathbf{n}}_j\right|^2 = 1$, then — $\overrightarrow{\mathbf{n}}_i \cdot \overrightarrow{\mathbf{n}}_j = 1 - \frac{1}{2}\left|\overrightarrow{\mathbf{n}}_i - \overrightarrow{\mathbf{n}}_j\right|^2$ — and (3.61) gets the form:

[19] We have disregarded all the terms of the order $\left|\overrightarrow{\mathbf{K}}_i\right|^2 \left|\overrightarrow{\mathbf{n}}_i - \overrightarrow{\mathbf{n}}_j\right|^2$, or inferior.

$$\vec{\mathbf{\Omega}}_i \cdot \vec{\mathbf{\Omega}}_j = \eta_i\eta_j - \frac{1}{2}\eta_i\eta_j \left|\vec{\mathbf{n}}_i - \vec{\mathbf{n}}_j\right|^2 + \frac{1}{s}\left(\eta_i \vec{\mathbf{n}}_i \cdot \vec{\mathbf{K}}_j + \eta_j \vec{\mathbf{n}}_j \cdot \vec{\mathbf{K}}_i\right) + \\ + \frac{1}{s^2}\left[\vec{\mathbf{K}}_i \cdot \vec{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j \left(\left|\vec{\mathbf{K}}_i\right|^2 + \left|\vec{\mathbf{K}}_j\right|^2\right)\right] + ... \tag{3.62}$$

Now, the **Assumption 2**, plus the fact that our lattice model involves only first-neighbor interactions, allow us to series expand the differences — $\vec{\mathbf{n}}_i - \vec{\mathbf{n}}_j$ — as follows[20]:

$$\vec{\mathbf{n}}_i - \vec{\mathbf{n}}_j = \sum_{l=1}^{d} x_{ij}^l \frac{\partial \vec{\mathbf{n}}}{\partial x^l}|_{\vec{\mathbf{x}}_i} + \frac{1}{2}\sum_{l,k=1}^{d} x_{ij}^k x_{ij}^l \frac{\partial^2 \vec{\mathbf{n}}}{\partial x^l \partial x^k}|_{\vec{\mathbf{x}}_i} + ... \tag{3.63}$$

If we use (3.63) and particularize for the case of a D-dimensional hypercubic lattice with parameter a, we get:

$$\left|\vec{\mathbf{n}}_i - \vec{\mathbf{n}}_j\right|^2 \approx \sum_{l=1}^{d} \left|\frac{\partial \vec{\mathbf{n}}}{\partial x^l}|_{\vec{\mathbf{x}}_i}\right|^2 x_{ij}^l + ... = a^2 \sum_{l=1}^{d} \left|\partial_l \vec{\mathbf{n}}(\tau, \vec{\mathbf{x}}_i)\right|^2 + ... \tag{3.64}$$

The cross-terms in (3.62) can be also expanded, respectively as:

$$\vec{\mathbf{n}}_i \cdot \vec{\mathbf{K}}_j = \vec{\mathbf{n}}_j \cdot \vec{\mathbf{K}}_j + \sum_{l=1}^{d} x_{ij}^l \frac{\partial \vec{\mathbf{n}}}{\partial x^l}|_{\vec{\mathbf{x}}_i} \cdot \vec{\mathbf{K}}_j + \frac{1}{2}\sum_{l,k=1}^{d} x_{ij}^k x_{ij}^l \frac{\partial^2 \vec{\mathbf{n}}}{\partial x^l \partial x^k}|_{\vec{\mathbf{x}}_i} \cdot \vec{\mathbf{K}}_j + ... \tag{3.65}$$

$$\vec{\mathbf{n}}_j \cdot \vec{\mathbf{K}}_i = \vec{\mathbf{n}}_i \cdot \vec{\mathbf{K}}_i - \sum_{l=1}^{d} x_{ij}^l \frac{\partial \vec{\mathbf{n}}}{\partial x^l}|_{\vec{\mathbf{x}}_i} \cdot \vec{\mathbf{K}}_j - \frac{1}{2}\sum_{l,k=1}^{d} x_{ij}^k x_{ij}^l \frac{\partial^2 \vec{\mathbf{n}}}{\partial x^l \partial x^k}|_{\vec{\mathbf{x}}_i} \cdot \vec{\mathbf{K}}_j + ... \tag{3.66}$$

Applying this to the $1/s$ term in (3.62), one gets[21]:

$$\sum_{\langle i,j\rangle}\left(\eta_i \vec{\mathbf{n}}_i \cdot \vec{\mathbf{K}}_j + \eta_j \vec{\mathbf{n}}_j \cdot \vec{\mathbf{K}}_i\right) = \sum_{\langle i,j\rangle}\eta_i\left(\vec{\mathbf{n}}_i \cdot \vec{\mathbf{K}}_j - \vec{\mathbf{n}}_j \cdot \vec{\mathbf{K}}_i\right) = 2\sum_i \eta_i \sum_{\vec{\delta}_i} \vec{\delta}_i \cdot \nabla \vec{\mathbf{n}}(\tau, \vec{\mathbf{x}}_i) + ... = 0 \tag{3.67}$$

And the last sum yields zero because it includes, for each vector $\vec{\delta}_i$, also its opposite.

Applying (3.64)-(3.67) to (3.62) and summing over the lattice, yields the following classical Hamiltonian of the D-dimensional system is given by:

[20] The continuum approximation will be equivalent to neglecting derivatives of $\vec{\mathbf{n}}$, of order larger than 1, in all the following expressions.

[21] The vectors $\vec{\delta}_i$ are the ones that connect the sit i to its nearest-neighbors.

$$
\begin{aligned}
Js^2 \sum_{\langle i,j\rangle\in\mathscr{L}} \overrightarrow{\mathbf{\Omega}}(\tau,\overrightarrow{\mathbf{x}}_i)\cdot\overrightarrow{\mathbf{\Omega}}(\tau,\overrightarrow{\mathbf{x}}_j) &= -2JNDs^2 - \frac{Js^2}{2}\sum_{\langle i,j\rangle\in\mathscr{L}}\eta_i\eta_j a^2\sum_{l=1}^{D}\left|\partial_l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}}_i)\right|^2 + \\
&\quad + J\sum_{\langle i,j\rangle\in\mathscr{L}}\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j\left(\left|\overrightarrow{\mathbf{K}}_i\right|^2+\left|\overrightarrow{\mathbf{K}}_j\right|^2\right)\right] = \\
&= E_{cl} + Js^2a^2D\sum_{i\in\mathscr{L}}\sum_{l=1}^{D}\left|\partial_l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}}_i)\right|^2 + \\
&\quad + J\sum_{\langle i,j\rangle\in\mathscr{L}}\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j\left(\left|\overrightarrow{\mathbf{K}}_i\right|^2+\left|\overrightarrow{\mathbf{K}}_j\right|^2\right)\right] = \qquad (3.68)
\end{aligned}
$$

Using the representation — $\sum_{i\in\mathscr{L}}A_i = a^{-D}\int d^D\overrightarrow{\mathbf{x}}\,A(\overrightarrow{\mathbf{x}})\sum_i\delta(\overrightarrow{\mathbf{x}}-\overrightarrow{\mathbf{x}}_i)$ — in (3.68), we get:

$$
E_{cl} + \frac{1}{2}\int d^D\overrightarrow{\mathbf{x}}\,\rho_s(\overrightarrow{\mathbf{x}})\sum_{l=1}^{D}\left|\partial_l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\right|^2 + J\sum_{\langle i,j\rangle\in\mathscr{L}}\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j\left(\left|\overrightarrow{\mathbf{K}}_i\right|^2+\left|\overrightarrow{\mathbf{K}}_j\right|^2\right)\right] \qquad (3.69)
$$

By defining $\rho_s(\overrightarrow{\mathbf{x}})$ as follows:

$$
\rho_s(\overrightarrow{\mathbf{x}}) \equiv 2Js^2a^{2-D}D\sum_{i\in\mathscr{L}}\delta^{(D)}(\overrightarrow{\mathbf{x}}-\overrightarrow{\mathbf{x}}_i) \qquad (3.70)
$$

To get the continuum approximation in the second term of (3.69), we just have to realize that $\rho_s(\overrightarrow{\mathbf{x}})$ is a translation invariant function and can be replaced by its spacial average:

$$
\overline{\rho}_s = \frac{1}{Na^D}\int d^D\overrightarrow{\mathbf{x}}\,\rho_s(\overrightarrow{\mathbf{x}}) = 2Js^2a^{2-D}D \qquad (3.71)
$$

We call this parameter - the **Stiffness Constant**. Finally, using Einstein's summation convention, the classical Hamiltonian takes the form:

$$
\mathcal{H}_{cl} = E_{cl} + \frac{\overline{\rho}_s}{2}\int d^D\overrightarrow{\mathbf{x}}\left[\partial_l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\cdot\partial^l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\right] + J\sum_{\langle i,j\rangle\in\mathscr{L}}\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j\left(\left|\overrightarrow{\mathbf{K}}_i\right|^2+\left|\overrightarrow{\mathbf{K}}_j\right|^2\right)\right] \qquad (3.72)
$$

To deal with the last term, we must express it as an integral in momentum-space. This is done in the [Appendix C.7] and we just quote the result (with $J_{ij} = J(\overrightarrow{\mathbf{x}}_j - \overrightarrow{\mathbf{x}}_i)$):

$$
\begin{aligned}
\sum_{i,j\in\mathscr{L}} J_{ij}\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_j - \frac{1}{2}\eta_i\eta_j\left(\left|\overrightarrow{\mathbf{K}}_i\right|^2+\left|\overrightarrow{\mathbf{K}}_j\right|^2\right)\right] &= \frac{Na_D}{(2\pi)^D}\int_{FBZ} d^D\overrightarrow{\mathbf{q}}\left(J(\overrightarrow{\mathbf{q}}) - J(\frac{\overrightarrow{\pi}}{a})\right)\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{-\overrightarrow{\mathbf{q}}} \\
&= \frac{1}{2}\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\chi^{-1}_{\overrightarrow{\mathbf{q}}}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{-\overrightarrow{\mathbf{q}}} \qquad (3.73)
\end{aligned}
$$

For $J(\overrightarrow{\mathbf{q}}) = \frac{1}{N}\sum_{\overrightarrow{\mathbf{x}}\in\mathscr{L}} J(\overrightarrow{\mathbf{x}})e^{i\overrightarrow{\mathbf{x}}\cdot\overrightarrow{\mathbf{q}}}$ and $\chi^{-1}_{\overrightarrow{\mathbf{q}}} = 2Na^D\left(J(\overrightarrow{\mathbf{q}}) - J(\frac{\overrightarrow{\pi}}{a})\right)$.

We then get the final result:

$$\mathcal{H}_{cl} = E_{cl} + \frac{\overline{\rho}_s}{2}\int d^D\overrightarrow{\mathbf{x}}\left[\partial_l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\cdot\partial^l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\right] + \frac{1}{2}\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\chi^{-1}_{\overrightarrow{\mathbf{q}}}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{-\overrightarrow{\mathbf{q}}} \tag{3.74}$$

3.3.2. Continuum Approximation of the Geometrical Berry Phase

The Berry phase $\omega[\overrightarrow{\mathbf{\Omega}}_i]$ is a functional that can be expressed in terms of a vector potential, as shown in (3.52) and (3.53). The vector potential, as defined in (3.52), has an even parity[22]:

$$\overrightarrow{\mathbf{A}}[-\overrightarrow{\mathbf{\Omega}}_i] = \overrightarrow{\mathbf{A}}[\overrightarrow{\mathbf{\Omega}}_i] \tag{3.75}$$

This means that we can perform the following manipulations:

$$s\sum_{j\in\mathscr{L}}\omega\left[\eta_j\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}}_j) + \frac{\overrightarrow{\mathbf{K}}(\tau,\overrightarrow{\mathbf{x}}_j)}{s}\right] = s\sum_{j\in\mathscr{L}}\int_0^\beta d\tau\overrightarrow{\mathbf{A}}_j\left[\eta_j\overrightarrow{\mathbf{n}}_j + \frac{\overrightarrow{\mathbf{K}}_j}{s}\right]\cdot\frac{d}{d\tau}\left[\eta_j\overrightarrow{\mathbf{n}}_j + \frac{\overrightarrow{\mathbf{K}}_j}{s}\right] = \tag{3.76}$$

$$= s\sum_{j\in\mathscr{L}}\eta_j\omega\left[\overrightarrow{\mathbf{n}}_j + \eta_j\frac{\overrightarrow{\mathbf{K}}_j}{s}\right] =$$

$$= \sum_{j\in\mathscr{L}}\left\{s\eta_j\omega\big[\overrightarrow{\mathbf{n}}_j\big] + \frac{\delta\omega\big[\overrightarrow{\mathbf{n}}_j\big]}{\delta\overrightarrow{\mathbf{\Omega}}}\cdot\overrightarrow{\mathbf{K}}_j + ...\right\} \tag{3.77}$$

It only remains to calculate the functional derivative — $\frac{\delta\omega}{\delta\overrightarrow{\mathbf{\Omega}}}$. The result is also derived in [Appendix C.7] and we quote it here, in its simplest form:

$$\delta\omega[\overrightarrow{\mathbf{\Omega}}_i] = \int_0^\beta d\tau\left(\overrightarrow{\mathbf{\Omega}}_i\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{\Omega}}_i\right)\cdot\delta\overrightarrow{\mathbf{\Omega}}_i \tag{3.78}$$

Meaning that (3.76) will be written as:

$$\sum_{j\in\mathscr{L}}s\eta_j\omega\big[\overrightarrow{\mathbf{n}}_j\big] + \sum_{i\in\mathscr{L}}\int_0^\beta d\tau\left(\overrightarrow{\mathbf{n}}_j(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}_j(\tau)\right)\cdot\overrightarrow{\mathbf{K}}_j(\tau) \tag{3.79}$$

The first term — $\Upsilon[\overrightarrow{\mathbf{n}}]$ — depends only in the main field and corresponds to the geometrical Berry phase associated with $\overrightarrow{\mathbf{n}}$. On the other hand, the second term can be written as a single integral over momentum-space, that goes as follows:

$$is\sum_{i\in\mathscr{L}}\omega[\overrightarrow{\mathbf{\Omega}}(\tau,\overrightarrow{\mathbf{x}}_i)] = i\Upsilon\big[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\big] + i\int_0^\beta d\tau\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{-\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}} + .. \tag{3.80}$$

[22] Note that the transformation $\overrightarrow{\mathbf{\Omega}}_i \to -\overrightarrow{\mathbf{\Omega}}_i$ is equivalent to $\theta_i \to \pi - \theta_i$ and $\hat{\phi} \to -\hat{\phi}$. Plugging this into the definition (3.52), we get the wanted invariance of the $\overrightarrow{\mathbf{A}}[\overrightarrow{\mathbf{\Omega}}_i]$.

3.3.3. Emergence of the Non-Linear Sigma Model

By gathering the results of the last two sections — (3.74) and (3.80) — we have the following approximation for the action:

$$S^D[\overrightarrow{\mathbf{n}},\overrightarrow{\mathbf{K}}] = i\Upsilon\left[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] + \frac{\overline{\rho}_s}{2}\int_0^\beta d\tau \int d^D\overrightarrow{\mathbf{x}}\left[\partial_l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\cdot\partial^l\overrightarrow{\mathbf{n}}(\tau,\overrightarrow{\mathbf{x}})\right] + \\ + \frac{1}{2}\int_0^\beta d\tau\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\left\{2i\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{-\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}} + \chi^{-1}_{\overrightarrow{\mathbf{q}}}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{-\overrightarrow{\mathbf{q}}}\right\} \tag{3.81}$$

The $\overrightarrow{\mathbf{K}}$- dependent part can be rewritten, by completing the square. The integrand is then equal to:

$$\left|\chi^{-1}_{\overrightarrow{\mathbf{q}}}\right|\left|\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}} + i\chi_{\overrightarrow{\mathbf{q}}}\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{-\overrightarrow{\mathbf{q}}}\right|^2 + \chi_{\overrightarrow{\mathbf{q}}}\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{-\overrightarrow{\mathbf{q}}}\cdot\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{\overrightarrow{\mathbf{q}}} \tag{3.82}$$

Putting this form in the full path-integral, we get[23]:

$$Z_D[\overrightarrow{\mathbf{n}},\overrightarrow{\mathbf{K}}] = \int\mathscr{D}\overrightarrow{\mathbf{n}}\exp\left[-i\Upsilon - \frac{\overline{\rho}_s}{2}\int_0^\beta d\tau\int d^D\overrightarrow{\mathbf{x}}\left[\partial_l\overrightarrow{\mathbf{n}}\cdot\partial^l\overrightarrow{\mathbf{n}}\right] - \right. \\ \left. -\frac{1}{2}\int_0^\beta d\tau\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\chi_{\overrightarrow{\mathbf{q}}}\left|\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{\overrightarrow{\mathbf{q}}}\right|^2\right]\times \\ \times\int\mathscr{D}\overrightarrow{\mathbf{K}}\exp\left[-\frac{1}{2}\int_0^\beta d\tau\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\left|\chi^{-1}_{\overrightarrow{\mathbf{q}}}\right|\left|\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}} + i\chi_{\overrightarrow{\mathbf{q}}}\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{-\overrightarrow{\mathbf{q}}}\right|^2\right] \tag{3.83}$$

Finally, the Gaussian integral over the canting field is independent of $\overrightarrow{\mathbf{n}}(\tau)$, which gives rise to an (irrelevant) multiplicative constant. Hence, the effective action for the $\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)$ field gets reduced to:

[23]Note that the change of variable $\hat{\Omega}\to\left(\overrightarrow{\mathbf{n}},\overrightarrow{\mathbf{K}}\right)$ is, to first order in $\left|\frac{\overrightarrow{\mathbf{K}}(\tau,\overrightarrow{\mathbf{x}}_j)}{s}\right|$, a linear transformation, which means that its Jacobian is a constant. Therefore, transformation of the measure from $\int\mathscr{D}\overrightarrow{\mathbf{\Omega}}$ to $\int\mathscr{D}\overrightarrow{\mathbf{n}}\mathscr{D}\overrightarrow{\mathbf{K}}$ consists only of a constant scale factor. Since all multiplicative constants in the Generating Functional are irrelevant, we will not even care about this constant scale factor.

$$
\begin{aligned}
S^D_{eff}[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)] &= i\Upsilon + \frac{\overline{\rho}_s}{2}\int_0^\beta d\tau \int d^D\overrightarrow{\mathbf{x}}\left[\partial_l \overrightarrow{\mathbf{n}}\cdot\partial^l\overrightarrow{\mathbf{n}}\right] + \\
&+ \frac{1}{2}\int_0^\beta d\tau \int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\chi_{\overrightarrow{\mathbf{q}}}\left|\left(\overrightarrow{\mathbf{n}}(\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau)\right)_{\overrightarrow{\mathbf{q}}}\right|^2 = \\
&= i\Upsilon + \frac{\overline{\rho}_s}{2}\int_0^\beta d\tau \int d^D\overrightarrow{\mathbf{x}}\left[\partial_l \overrightarrow{\mathbf{n}}\cdot\partial^l\overrightarrow{\mathbf{n}}\right] + \\
&+ \frac{1}{2}\int_0^\beta d\tau \int d^D\overrightarrow{\mathbf{x}}\,\chi_{\overrightarrow{\mathbf{0}}}\left|\left(\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right)\right|^2
\end{aligned}
\tag{3.84}
$$

The last step deserves some comments: First of all, if the interactions are local enough, the function $J(\overrightarrow{\mathbf{q}})$ will also be approximately constant for the allowed values of $\overrightarrow{\mathbf{q}}$. Hence, we can approximate $\chi^{-1}_{\overrightarrow{\mathbf{q}}} \approx \chi^{-1}_{\overrightarrow{\mathbf{0}}} = 2Na^D\left(J(\overrightarrow{\mathbf{0}}) - J(\frac{\overrightarrow{\pi}}{a})\right)$. In particular, for the Heisenberg model, we have:

$$\chi^{-1}_{\overrightarrow{\mathbf{0}}} = 8Da^D J$$

Finally, the use of the **Parseval-Plancheret Formula** — $\int \frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\left|f(\overrightarrow{\mathbf{q}})\right|^2 = \int d^D\overrightarrow{\mathbf{x}}\left|f(\overrightarrow{\mathbf{x}})\right|^2$— allows us to turn the integral over momentum-space into the integral in real-space, that appears in (3.84).

Furthermore, the equation (3.84) can be simplified by realizing the following identity[24]:

$$\left|\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right|^2 = \left|\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right|^2 \tag{3.85}$$

Using it, we get:

$$S^D_{eff}[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)] = i\Upsilon\left[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] + \frac{\overline{\rho}_s}{2}\int_0^\beta d\tau\int d^D\overrightarrow{\mathbf{x}}\left\{\left[\partial_l\overrightarrow{\mathbf{n}}\cdot\partial^l\overrightarrow{\mathbf{n}}\right] + \frac{\chi_{\overrightarrow{\mathbf{0}}}}{\overline{\rho}_s}\left|\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right|^2\right\} \tag{3.86}$$

By defining a **characteristic velocity** $c = \sqrt{\frac{\overline{\rho}_s}{\chi_{\overrightarrow{\mathbf{0}}}}}$ and adopting the 4-vector notation - $\left(x^0, x^1, ..., x^D\right) = \left(c\tau, \overrightarrow{\mathbf{x}}\right)$, we arrive at the following beautiful form:

$$S^D_{eff}[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)] = i\Upsilon\left[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] + \frac{\overline{\rho}_s}{2c}\int_0^{c\beta} dx^0\int d^D\overrightarrow{\mathbf{x}}\left[\partial_\mu\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\cdot\partial_\mu\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right];\quad \left|\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right|^2 = 1 \tag{3.87}$$

Apart from the first term (which is a topological term, as will be seen in the next section), the effective Quantum Field Theory that describes the Néel magnetization for the D**-dimensional AFM**

[24] Which is easily proved by noticing that $\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\perp\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)$.

Heisenberg Model is the (Lorentz and $\mathcal{O}(3)$-invariant) **Non-Linear Sigma Model (NLSM) in a $(D+1)$-dimensional space**[25]. The corresponding action is:

$$S^D_{NLSM}[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)] = \frac{\Lambda^{1-D}}{2g}\int_0^{c\beta} dx^0 \int d^D\overrightarrow{\mathbf{x}}\,\left[\partial_\mu \overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\cdot\partial_\mu \overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] \tag{3.88}$$

The dimensionless coupling parameter is given by $g = \frac{c}{\overline{\rho}_s}\Lambda^{1-D}$, where Λ represents the small-distance cut-off, which must be larger than the original lattice parameter. This coupling parameter is given by:

$$g_{s,D}(\Lambda) = \frac{2}{s}\left(\frac{a}{\Lambda}\right)^{D-1} \underset{s\to+\infty}{\longrightarrow} 0 \tag{3.89}$$

From which we conclude that **The Model is Weakly-Coupled in the Classical Limit**.

3.4. One-Dimensional Models: The Θ-Term Topological Action

References: [6,7,23]

We have derived the effective Quantum Field Theory that describes the long-wavelength behavior of the Néel magnetization for the Heisenberg Model in D-dimensions. With it, came the realization that the action reduced to the well-known NLSM, plus an additional geometrical phase. In $D=1$, this phase can be calculated, in the continuum-limit, as follows:

$$\Upsilon\left[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] = \sum_{j=-\infty}^{\infty} s\eta_j\omega\left[\overrightarrow{\mathbf{n}}_j\right] = s\sum_{j=-\infty}^{\infty}\left\{\omega\left[\overrightarrow{\mathbf{n}}_{2j}\right]\text{-}\omega\left[\overrightarrow{\mathbf{n}}_{2j-1}\right]\right\} = \tag{3.90}$$

$$= s\int_{-\infty}^{\infty} dx \frac{\delta\omega}{\delta\overrightarrow{\mathbf{n}}}\cdot\frac{\partial}{\partial x}\overrightarrow{\mathbf{n}}(\tau,x) = \frac{s}{2}\int_0^\beta d\tau\int_{-\infty}^{\infty} dx\left(\overrightarrow{\mathbf{n}}(\tau,x)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau,x)\right)\cdot\frac{\partial}{\partial x}\overrightarrow{\mathbf{n}}(\tau,x) \tag{3.91}$$

If we now define the following functional:

$$\Theta[\overrightarrow{\mathbf{n}}(\tau,x)] \equiv \frac{1}{4\pi}\int_0^\beta d\tau\int_{-\infty}^{\infty} dx\left(\overrightarrow{\mathbf{n}}(\tau,x)\times\frac{\partial}{\partial\tau}\overrightarrow{\mathbf{n}}(\tau,x)\right)\cdot\frac{\partial}{\partial x}\overrightarrow{\mathbf{n}}(\tau,x) \tag{3.92}$$

We can write:

$$\Upsilon\left[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] = 2\pi s\Theta[\overrightarrow{\mathbf{n}}(\tau,x)] \tag{3.93}$$

[25] For a finite temperature, the x^0 variable is periodic, with period βc. If we wish to describe the $T=0$ physics of the Heisenberg AFM, then we take the following limit:

$$\int_0^{c\beta} dx^0(...) = \int_{-c\beta/2}^{c\beta/2} dx^0(...) \to \int_{-\infty}^{\infty} dx^0(...)$$

Which means that the zero temperature AFM, in the thermodynamic limit, is described by the $\mathcal{O}(3)$-NLSM in a $(D+1)$-dimensional infinite Euclidean Space.

And the $D = 1$ effective action is just:

$$S_{eff}^{D=1}[\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)] = 2\pi i s \Theta[\overrightarrow{\mathbf{n}}(\tau,x)] + \frac{1}{2g_{s,D=1}(\Lambda)} \int\int dx^0 dx^1 \left[\partial_\mu \overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau) \cdot \partial^\mu \overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right] \tag{3.94}$$

This last result was first derived by Haldane [23], and it emphasizes that the Berry phase gets reduced to a so-called **Topological Θ-term** (or also Topological Angle). This term, as written in (3.92), is easily interpreted as being the number of times the image of the map:

$$\begin{aligned} \overrightarrow{\mathbf{n}}(\tau,x) : [-\frac{\beta c}{2}, \frac{\beta c}{2}[\times[-L,+L[&\to S^2 \\ (\tau,x) \quad &\to \hat{\Omega}(\tau,x) \end{aligned} \tag{3.95}$$

Wraps around the 2-sphere.

If both τ and x are chosen as periodic variables (i.e. finite temperature + PBC), then the value of $\Theta[\overrightarrow{\mathbf{n}}(\tau,x)]$ is always an integer, and depends only on the 2^{nd} homotopy class of the field configuration. This conclusion is also true, even if we are at $T = 0$ or in the thermodynamic limit ($L \to \infty$), provided that the field configurations have the same asymptotic limit in both directions. All in all, this term is a topological invariant of the field configuration.

Furthermore, since $\Theta[\overrightarrow{\mathbf{n}}(\tau,x)]$ is always an integer, obviously it **yields a trivial phase for the cases when s is an integer**. In such cases, the effective action of the Néel field will be given exactly, by the simple $O(3)$-NLSM in a two-dimensional space. I.e.

$$Z_{D=1}^{s\ integer} = \int \mathscr{D}\overrightarrow{\mathbf{n}}(\tau,x)\delta(\left|\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right|^2 - 1) \exp\left[-\frac{1}{2g_{s,D=1}(\Lambda)} \int_0^{\beta c}\int_\Lambda dx^0 dx^1 \left[\partial_\mu \overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau) \cdot \partial^\mu \overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}},\tau)\right]\right] \tag{3.96}$$

This last identification is widely known as the **Haldane Mapping**. The coupling parameter, as in the general case, goes as $1/s$.

3.5. The Haldane Conjecture

References: [6,7,23,24,25,27]

Using the Haldane Mapping, we have devised a way of studying the Heisenberg chain, for integer spins, using field-theoretical methods (in 2-dimensions). In this section, we will make use of **Wilson's Renormalization Group Theory**, to study some important properties of the $O(3)$-NLSM. In particular, we will derive an expression for the long-range spin-correlations, prove that there is a finite correlation-length and also a finite mass-gap on the low-energy spectrum for this model.

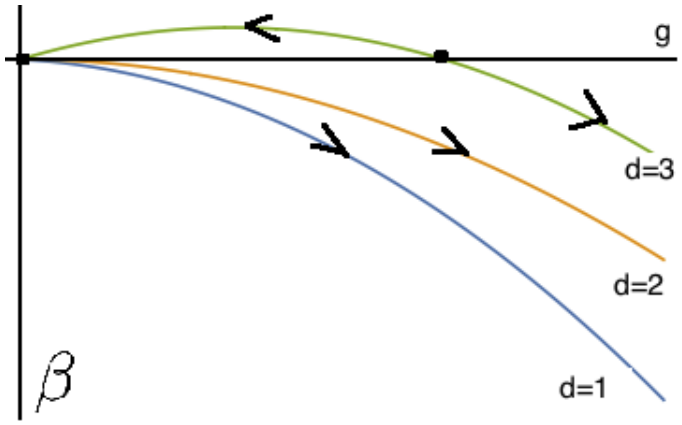


Figure 3.2.: Plot of the Polyakov β-function for the $O(3)$-NLSM in $d = 1, 2, 3$ dimensions. The direction of the renormalization flow is also marked by arrows.

3.5.1. Polyakov Renormalization Group (a Short Review)

References: [24]

This study was first done by A. M. Polyakov in 1975 [24, 25], when he built a renormalization group procedure by integrating iteratively the high-momentum modes of the $\overrightarrow{\mathbf{n}}$-field, using perturbation theory. A detailed and pedagogical description of this method can be found in [7, 24], but the important conclusion is encapsulated in the RG evolution of the coupling parameter g.

This one was found to be described by the following β-function (for a d-dimensional model)[26]:

$$\beta^d(g) \equiv \frac{dg}{d\ln(b)} = (d-2)g - \frac{1}{\zeta_d}g^2 + \mathcal{O}(g^4) \tag{3.97}$$

Where the rescaling transformation is ruled by the parameter $0 \ll b < 1$, as $x \to \widetilde{x} = b^{-1}x$.[27] The function (3.97) is plotted in the Figure 3.2, for the cases $d = 1, 2, 3$.

For $d = 2$, g is dimensionless — it is a **marginal parameter**. However, the lowest-order loop corrections cause this parameter to be renormalized and yields a negative beta function near $g = 0$. Consequently, the small-coupling NLSM is an IR-unstable fixed-point of the RG-flow and the macroscopic physics will be dominated by a large value of g.

By itself, the negativity of the β-function[28] means that the stable phase will be a disordered one. Nevertheless, we can draw more compelling conclusions from (3.97), by using it to derive an expression for the correlation length in the IR-limit.

To do that, we start by assuming that there is an universal length — ξ — that appears in the correlation function of the Néel field, as follows:

$$\frac{1}{V}\int \frac{d^2\overrightarrow{\mathbf{q}}}{4\pi^2}\left\langle \delta\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{0}})\cdot\delta\overrightarrow{\mathbf{n}}(\overrightarrow{\mathbf{x}})\right\rangle e^{i\overrightarrow{\mathbf{q}}\cdot\overrightarrow{\mathbf{x}}} = \left\langle \delta\overrightarrow{\mathbf{n}}_{\overrightarrow{\mathbf{q}}}\cdot\delta\overrightarrow{\mathbf{n}}_{-\overrightarrow{\mathbf{q}}}\right\rangle \approx \frac{constant}{\left|\overrightarrow{\mathbf{q}}\right|^2 + \xi_d^{-2} + ...} \tag{3.98}$$

[26] The first term in (3.97) comes from the rescaling tranformation, while the last comes from the lowest-order loop correction. By definition - $\zeta_1 = \pi$, $\zeta_2 = 2\pi$, $\zeta_3 = 2\pi^2$

[27] **Important Note:** From the above definition of the β-function, it is also easily seen that, as we move our renormalized theory to the IR (by increasing the small distance cut-off), the coupling will increase (if $\beta < 0$) or decrease (if $\beta > 0$).

[28] A property that is usually called 'Asymptotic Freedom' in high-energy physics.

Now, the crucial argument relies on the universality of ξ, which means that this distance will be the same, whether it is calculated in the original or renormalized theory. This can be expressed in the following equality (where Λ is the original small-length cut-off, $\tilde{\Lambda}$ is a renormalized cut-off and μ is a macroscopic length scale):

$$\xi_d[\mu, g(\mu)] = \xi_d[\tilde{\Lambda}; g(\widetilde{\Lambda})] \Rightarrow \frac{\mu}{\Lambda}\phi[g(\mu)] = \frac{\tilde{\Lambda}}{\Lambda}\phi[g(\widetilde{\Lambda})] \tag{3.99}$$

By dimensional analysis, ϕ is a function that only depends on the cut-off via the renormalized coupling parameter. Differentiating this equation with respect to $\ln(\Lambda/\tilde{\Lambda})$, one gets:

$$0 = \frac{\partial \frac{\tilde{\Lambda}}{\Lambda}}{\partial \ln\left(\frac{\Lambda}{\tilde{\Lambda}}\right)}\phi(g(\widetilde{\Lambda})) + \beta^d(g)\frac{\partial \xi_d}{\partial g} = -\xi_d(g) + \beta^d(g)\frac{\partial \xi_d}{\partial g} \tag{3.100}$$

The differential equation (3.100) is separable and easily solved. The general solution is:

$$\int_{g_0}^{g} \frac{dg}{\beta^d(g)} = \int_{\xi_0}^{\xi} \frac{d\xi_d}{\xi_d(g)} \tag{3.101}$$

For $d = 2$, the final result will be:

$$\xi_2(g) = c \times e^{\frac{2\pi}{g}} \tag{3.102}$$

A result which simply means that ξ_2 flows along with the RG, without ever going to zero. In other words, if we start in the disordered phase (for large-g, where ξ_2 is finite), we can flow backwards and conclude that ξ_2 remains finite for all the renormalized models.

3.5.2. The Haldane Spectral Gap

The main conclusion of the analysis done above can be summarized in the following statement:

- At zero temperature, the 2-point correlation function between field fluctuations decays exponentially with the distance. This can be seen by calculating the inverse Fourier transform of the expression (3.100), which goes as follows:

$$\begin{aligned}\left\langle \delta\overrightarrow{\mathbf{n}}(0)\cdot\delta\overrightarrow{\mathbf{n}}(x)\right\rangle &= \frac{1}{4\pi^2}\int_0^{+\infty} dq \frac{Cq}{q^2+\xi^{-2}}\int_0^{2\pi} d\theta e^{-iqr\cos\theta} = \\ &= \frac{C}{4\pi^2}\int_0^{+\infty} dk \frac{k}{k^2+\left(\frac{r}{\xi}\right)^2}\int_0^{2\pi} d\theta e^{-ik\cos\theta}\end{aligned} \tag{3.103}$$

The integral — $(1/2\pi)\int_0^{2\pi} d\theta e^{-ik\cos\theta} = J_0(k)$ — is a Bessel function of the first kind, so the only integral we need to deal with is of the form:

$$\frac{1}{2\pi}\int_0^{+\infty} dk \frac{kJ_0(k)}{k^2+a^2} = \frac{1}{2\pi}K_0(a) \underset{a\to+\infty}{\longrightarrow} \frac{1}{2\sqrt{2\pi}}\frac{e^{-a}}{\sqrt{a}}\left\{1-\frac{1}{8a}+...\right\} \tag{3.104}$$

At last, we can take this asymptotic expansion and replace $a \to {}^{r}/_{\xi}$, obtaining[29]:

$$\left\langle \delta\overrightarrow{\mathbf{n}}(0)\cdot\delta\overrightarrow{\mathbf{n}}(x)\right\rangle_{D=1} \propto \frac{e^{-\frac{|x|}{\xi_2}}}{\sqrt{|x|}}\left(1-\frac{\xi_2}{8\,|x|}+...\right) \tag{3.105}$$

Where $|x| = \sqrt{c^2\tau^2+x^2}$.

Our final important result is summarized in (3.105), but still some comments are now in order:

1. **The appearance of a length scale in the two-dimensional model is a purely quantum effect**, that appears only when loop-corrections are taken into account. In other words, it is a dynamical effect;
2. The correlations between the field fluctuations, at equal times, **decay with distance**. This is just the expression of the fact that **the zero-temperature phase of the 1-D Heisenberg AFM is disordered**;
3. The correlations for fluctuations at the same point in space, also **decay with imaginary time**. The interpretation of this is not as clear as the previous ones, but still it can be clarified as follows:

Let $|0\rangle$ be the vacuum state for the $\overrightarrow{\mathbf{n}}$ model and $|\Psi_m\rangle$ a complete set of exact energy eigenstates for the field Hamiltonian. Then the 2-point function — $\left\langle \delta\overrightarrow{\mathbf{n}}(x,0)\cdot\delta\overrightarrow{\mathbf{n}}(x,\tau)\right\rangle$ — can be expanded as follows:

$$\left\langle \delta\overrightarrow{\mathbf{n}}(x,0)\cdot\delta\overrightarrow{\mathbf{n}}(x,\tau)\right\rangle = \sum_{m\neq 0}\frac{\langle\Psi_0|\,\delta\overrightarrow{\mathbf{n}}(x,0)\,|\Psi_m\rangle\cdot\langle\Psi_m|\,\delta\overrightarrow{\mathbf{n}}(x,\tau)\,|\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle} \tag{3.106}$$

Since $\delta\overrightarrow{\mathbf{n}}(x,\tau)$ is an Heisenberg operator, it is written as — $\delta\overrightarrow{\mathbf{n}}(x,\tau) = e^{-H\tau}\delta\overrightarrow{\mathbf{n}}(x,0)e^{H\tau}$. Plugging this into equation (3.106), we get:

$$\left\langle \delta\overrightarrow{\mathbf{n}}(x,0)\cdot\delta\overrightarrow{\mathbf{n}}(x,\tau)\right\rangle = \sum_{m\neq 0}\frac{\left|\langle\Psi_0|\,\delta\overrightarrow{\mathbf{n}}(x,0)\,|\Psi_m\rangle\right|^2}{\langle\Psi_0\mid\Psi_0\rangle}e^{-\tau(E_m-E_0)} \tag{3.107}$$

Now, the expression (3.107) indicates that the decay of $\left\langle \delta\overrightarrow{\mathbf{n}}(x,0)\cdot\delta\overrightarrow{\mathbf{n}}(x,\tau)\right\rangle$ with imaginary time, is dominated by $e^{-\Delta\tau}$, where $\Delta = \min_m[E_m - E_0]$. Hence, we conclude that the decay of correlations with imaginary time **is a reflection of a spectral gap above the ground-state**[30]. This last statement is known as the **Haldane Conjecture** and it is believed to be applicable to all the Heisenberg chains, with integer localized spins. Obviously, the applicability of these results to the actual lattice systems is questionable, since the whole theory is built on a continuum approximation that is only

[29] The so-called 'Ornstein-Zernike' correlation function for a two-dimensional classical interacting gas.

[30] This gap, plus the knowledge that the ground-state is isotropic [Ch. 2] is enough to conclude that the Heisenberg AFM is disordered at $T = 0$. Otherwise, it would violate Goldstone's Theorem.

justifiable for $s \to +\infty$. Nevertheless, there is a strong numerical evidence that this conjecture remains valid, even when is as low as $s = 1$ [6,7,23,24].

For the half-integer spins this gap seems to be destroyed by the effect of the alternating topological phase (according to the Lieb-Schultz-Mattis Theorem). Some relevant discussions about these cases can be found in [6,27], but this was not explored in any way, by the author.

[This page was intentionally left blank]

4. Exactly Solvable Quantum Spin Models

We have seen so far that the $O(3)$-symmetric antiferromagnetic models are highly non-trivial to solve. In fact, the simplest Heisenberg Model with nearest-neighbor couplings is only exactly solved for the spin-1/2 one-dimensional case (Bethe Ansatz solution [6,7,38]). For any other bipartite lattice and spin multiplicity, we have established (in Chapter 2) that the structure of the (unique) manybody ground-state is of the utter most complexity, being almost impossible to describe in terms of product states.

In this chapter, we will see that there are AFM quantum spin models with cleverly built Hamiltonians, that allow the construction of their exact ground-state wavefunctions and the rigorous proof of important qualitative features of its low-energy spectrum (in particular, the existence of a gap in the thermodynamic limit). Knowledge about these alternative models, allows for some qualitative understanding of the physics behind the Heisenberg Model, by comparison [6].

4.1. The Majumdar-Ghosh Model

References: [7,28,29,32]

The first model to be explored consists of a (length N) spin-1/2 chain with nearest- and next-nearest-neighbor antiferromagnetic interactions. This model was first studied (numerically) by C. K. Majumdar and D. K. Ghosh in [28, 29], as part of an interesting class of frustrated AFM models in one-dimension. It is ruled by the following Hamiltonian (with $J > 0$):

$$H_{MG}^{N} = J \sum_{i=2}^{N-2} \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + \frac{J}{2} \left[\sum_{i=1}^{N-2} \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+2} + \overrightarrow{\mathbf{S}}_1 \cdot \overrightarrow{\mathbf{S}}_2 + \overrightarrow{\mathbf{S}}_{N-1} \cdot \overrightarrow{\mathbf{S}}_N \right] \tag{4.1}$$

By imposing the periodic boundary conditions (PBC) — $\overrightarrow{\mathbf{S}}_{N+1} = \overrightarrow{\mathbf{S}}_1$ and $\overrightarrow{\mathbf{S}}_{N+2} = \overrightarrow{\mathbf{S}}_2$ — we can rewrite (4.1) in the more natural form:

$$H_{MG}^{N,PBC} = J \sum_{i=1}^{N} \left[\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + \frac{1}{2} \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+2} \right] \tag{4.2}$$

4.1.1. Building the Exact Ground-State

Despite its apparent complexity, the ground-states of (4.2) can be explicitly written down by noticing that the terms in sum are actually projectors onto the highest-spin subspace, for each trio of consecutive

spins. To see this, we must consider a trio of spins-1/2 localized in the sites i, $i+1$ and $i+2$, about which we know that:

1. The Hilbert space - $\mathscr{H}_i$ - of this subsystem is 8-dimensional;
2. The total Spin Operator for this trio is given by $\overrightarrow{\mathbf{S}}_{Tot} = \overrightarrow{\mathbf{S}}_i + \overrightarrow{\mathbf{S}}_{i+1} + \overrightarrow{\mathbf{S}}_{i+2}$;
3. By the **Addition Theorem for Angular Momenta**, $\mathscr{H}_i$ can be decomposed into eigensubspaces of S^2_{Tot}, as follows:

$$\mathscr{H}_i = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2} \tag{4.3}$$

The projector onto the $J = 3/2$ subspace — designated as $P_{3/2}(i, i+1, i+2)$ — can be written in terms of the individual spin operators[1]:

$$P_{3/2}(i, i+1, i+2) = \frac{1}{3}\left(S^2_{Tot} - \frac{3}{4}\right) = \frac{1}{2} + \frac{2}{3}\left[\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+2} + \overrightarrow{\mathbf{S}}_{i+1} \cdot \overrightarrow{\mathbf{S}}_{i+2}\right] \tag{4.4}$$

If we perform the sum over the N sites in the chain (with PBC), we get:

$$\sum_{i=1}^{N} P_{3/2}(i, i+1, i+2) = \frac{N}{2} + \frac{4}{3}\sum_{i=1}^{N}\left[\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + \frac{1}{2}\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+2}\right] \tag{4.5}$$

And from (4.5), it is clear that we can write (4.2) as follows [2]:

$$H^{N,PBC}_{MG} = \frac{3J}{4}\sum_{i=1}^{N} P_{3/2}(i, i+1, i+2) - \frac{3JN}{8} \tag{4.6}$$

Since every projector is a non-negative operator, we know that all the eigenenergies of (4.2) must obey the inequality — $\epsilon \geq -\frac{3JN}{8}$. Hence, if we can find states $|\psi\rangle$ which obey $P_{3/2}(i, i+1, i+2)\,|\psi\rangle = 0$, for each $i \in \{1, ..., N\}$, those will be ground-states of the full Hamiltonian.

This later condition can be fullfilled if we manage to build a wavefunction without any component with total spin 3/2, for each trio of spins in the chain. Given a trio of consecutive spins, there are two ways of doing this:

$$\left|\phi^i_1(m)\right\rangle = |1/2, m\rangle_i \otimes \frac{1}{\sqrt{2}}\left[|\uparrow\rangle_{i+1}|\downarrow\rangle_{i+2} - |\downarrow\rangle_{i+1}|\uparrow\rangle_{i+2}\right] \tag{4.7}$$

or

$$\left|\phi^i_2(m)\right\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle_i|\downarrow\rangle_{i+1} - |\downarrow\rangle_i|\uparrow\rangle_{i+1}\right] \otimes |1/2, m\rangle_{i+2} \tag{4.8}$$

[1] This is easily verified to be true, since $\frac{1}{3}\left(S^2_{Tot} - \frac{3}{4}\right)|1/2, m\rangle = 0$ and $\frac{1}{3}\left(S^2_{Tot} - \frac{3}{4}\right)|3/2, m\rangle = |3/2, m\rangle$.

[2] The same reasoning can be applied to obtain the open chain Hamiltonian, but one must sum only for the first $N-2$ sites, instead of N. This yields:

$$H^N_{MG} = \frac{3J}{4}\sum_{i=1}^{N-2} P_{3/2}(i, i+1, i+2) - \frac{3J(N-2)}{8}$$

So, to build a full manybody ground-state, we must pair up the consecutive spins into singlets ($J = 0$) alternately along the chain, and consider the tensor product of all those singlets. Obviously, there will be several ways to pair up the spins, and therefore the ground-state will no longer be unique.

To better represent the states (4.7) and (4.8), we introduce the following index notation, invented by I. Affleck, T. Kennedy, E. Lieb and H. Tasaki in [32] (the Einstein's summation convention over greek indices will be assumed thereafter)[3]:

$$\psi_{\alpha}^{(i)} = \left(|\uparrow\rangle_i, |\downarrow\rangle_i\right) \quad \text{and} \quad \psi^{(i)\alpha} \equiv \epsilon^{\alpha_i\beta}\psi_{\beta} = \left(|\downarrow\rangle_i, -|\uparrow\rangle_i\right) \tag{4.9}$$

Which means, for example, that:

$$|\uparrow\rangle_i |\downarrow\rangle_{i+1} - |\downarrow\rangle_i |\uparrow\rangle_{i+1} = \psi_{\alpha}^{(i)}\psi^{(i+1)\alpha} \equiv \psi_{\alpha}^{\ \alpha}$$

In all of the following discussion, the site index — (i) — will be suppressed since it will be clear, from the position of the greek index, to which site is it referring.

In this new notation, the (non-normalized) states (4.7) and (4.8) can be represented simply as $|\phi_1(\alpha)\rangle = \psi_{\alpha}\psi_{\beta}^{\ \beta}$ and $|\phi_2(\alpha)\rangle = \psi_{\beta}^{\ \beta}\psi_{\alpha}$. They can also be given an useful graphical representation, as shown in the Figure 4.1. Generalizing this procedure for the whole lattice, it is easy to write down **the ground-states of the full Majumdar-Ghosh Hamiltonian**, as follows:

- Open Chain with an even number of sites (5 different ground-states):

$$\Psi_1 = \psi_{\alpha_1}^{\ \alpha_1} \otimes ... \otimes \psi_{\alpha_{N/2}}^{\ \alpha_{N/2}} \tag{4.10}$$

$$\Psi_{2\ \beta}^{\ \ \alpha} = \psi^{\alpha} \otimes \psi_{\alpha_1}^{\ \alpha_1} \otimes ... \otimes \psi_{\alpha_{(N-2)/2}}^{\ \alpha_{(N-2)/2}} \otimes \psi_{\beta} \tag{4.11}$$

- Chain (Open or Periodic) with an odd number of sites (4 different ground-states):

$$\Psi_{1\ \alpha} = \psi_{\alpha_1}^{\ \alpha_1} \otimes ... \otimes \psi_{\alpha_{(N-1)/2}}^{\ \alpha_{(N-1)/2}} \otimes \psi_{\alpha} \tag{4.12}$$

$$\Psi_{2\ \alpha} = \psi_{\alpha} \otimes \psi^{\alpha_1}_{\ \alpha_1} \otimes ... \otimes \psi^{\alpha_{(N-1)/2}}_{\ \ \alpha_{(N-1)/2}} \tag{4.13}$$

- Periodic Chain with an even number of sites (2 different ground-states):

$$\Psi_1^{PBC} = \psi_{\alpha_1}^{\ \alpha_1} \otimes ... \otimes \psi_{\alpha_{N/2}}^{\ \alpha_{N/2}} \tag{4.14}$$

$$\Psi_2^{PBC} = \Psi_{2\ \beta}^{\ \ \beta} = \psi^{\beta} \otimes \psi_{\alpha_1}^{\ \alpha_1} \otimes ... \otimes \psi_{\alpha_{(N-2)/2}}^{\ \alpha_{(N-2)/2}} \otimes \psi_{\beta} \tag{4.15}$$

The states (4.10)-(4.15) are also represented graphically in Figure 4.1.

For the translation invariant cases — Periodic and Infinite Chain — the ground-states (4.14)-(4.15) are found to break the lattice translation symmetry — they are **Dimerized States**. Still, one can

[3]By definition, the symbol $\epsilon^{\alpha\beta}$ stand for the anti-symmetrical tensor — $\epsilon^{12} = -\epsilon^{21} = 1$ and $\epsilon^{11} = \epsilon^{22} = 0$.

choose a new basis for the ground-state manifold containing only elements that are invariant under lattice translations. A possible choice is shown in (4.16)[4]:

$$\Phi^{\pm} = \frac{1}{\sqrt{2}} \left(\Psi_1^{PBC} \pm \Psi_2^{PBC} \right) \tag{4.16}$$

These symmetrical states are commonly called **Resonating Valence-Bond** (RVB) states, since they have a striking similarity with the electronic states in Benzene rings.

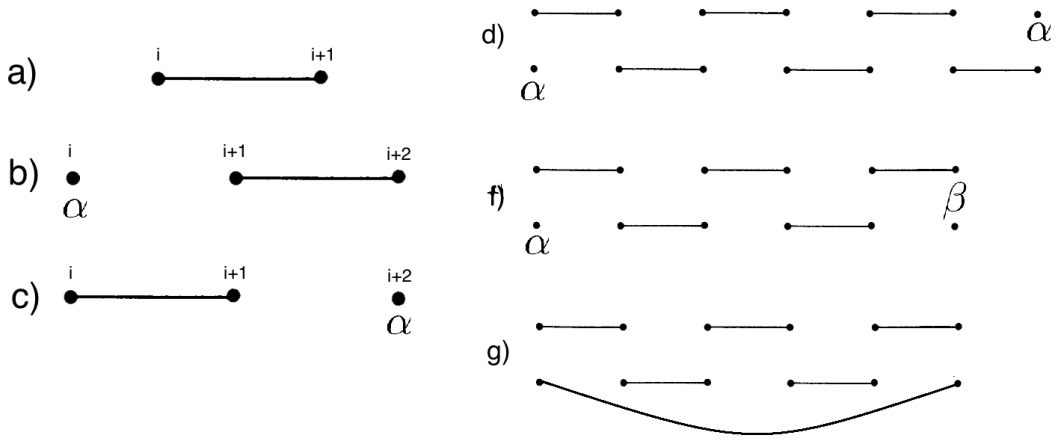


Figure 4.1.: Diagramatics of the Majumdar-Ghosh ground-states: **a)** Representation of a singlet state ψ_α^α; **b)** State $|\phi_1(\alpha)\rangle = \psi_\alpha \psi_\beta^{\ \beta}$; **c)** State $|\phi_2(\alpha)\rangle = \psi_\beta^{\ \beta} \psi_\alpha$; **d)** Ground-states of the even chain; **e)** Ground-states of the even chain and **f)** Ground-states of the Periodic chain with an even number of sites.

4.1.2. Order and Correlations in the Ground-State

In this section, we antecipate that the only ground-states of the MG model (in the thermodynamic limit) will be the ones defined in (4.16) and we will only consider those, for now. The first thing one notices is that both $\Phi^{\pm}$ are singlets of the total spin operator, simply because they are linear combinations of tensor product of neighboring spin singlets:

$$S_{Tot}^2 \Phi^{\pm} = 0 \Longrightarrow \left[\frac{1}{N} \sum_{i=1}^{N} \overrightarrow{\mathbf{S}}_i \right] \Phi^{\pm} = 0 \tag{4.17}$$

So, the ground-state is not magnetized[5]. But, is there some kind of Neél order in this case (even if it is only at short length scales)? To answer this, we must calculate the spin-spin correlation function in each one of the states (4.16), and that will require the development of some useful formalism.

We begin by defining **the inner-product of local spin states**, using the index language defined above:

[4]Since $\mathbb{T}\Psi_2^{PBC} = \Psi_1^{PBC}$, and $\mathbb{T}\Psi_1^{PBC} = \Psi_2^{PBC}$, with $\mathbb{T}$ being the translation operator of one lattice spacing, it is obvious that $\Phi^{\pm}$ are invariant under any lattice translation.

[5]Which does not mean necessarily, that there is null magnetization in the thermodynamic limit, at zero temperature. Remember the discussion about long-range order in Chapter 2.

$$(\psi_\alpha, \psi_\beta) = \delta_{\alpha\beta} \quad \left(\psi^\alpha, \psi^\beta\right) = \epsilon^{\alpha\mu}\epsilon^{\beta\nu}\left(\psi_\mu, \psi_\nu\right) = \delta^{\alpha\beta} \quad \left(\psi_\alpha, \psi^\beta\right) = \epsilon^{\beta\gamma}\delta_{\gamma\alpha} = \epsilon^\beta_\alpha \tag{4.18}$$

$$\left(\psi_\alpha^{\ \beta}, \psi_\gamma^{\ \delta}\right) = \epsilon^{\beta\mu}\epsilon^{\delta\nu}\left(\psi_\alpha, \psi_\gamma\right)\left(\psi_\mu, \psi_\nu\right) = \delta_{\alpha\gamma}\delta^{\beta\delta} \tag{4.19}$$

Using these facts, we can start by calculating directly the norms of Ψ_1^{PBC} and Ψ_2^{PBC}, as follows[6]:

$$\left(\Psi_1^{PBC}, \Psi_1^{PBC}\right) = \left(\Psi_2^{PBC}, \Psi_2^{PBC}\right) = \left(\psi_{\alpha_1}^{\ \alpha_1}, \psi_{\beta_1}^{\ \beta_1}\right) ... \left(\psi_{\alpha_{N/2}}^{\ \alpha_{N/2}}, \psi_{\beta_{N/2}}^{\ \beta_{N/2}}\right) = \delta_{\alpha_1}^{\ \alpha_1} ... \delta_{\alpha_{N/2}}^{\ \alpha_{N/2}} = 2^{N/2} \tag{4.20}$$

$$\begin{aligned}\left(\Psi_1^{PBC}, \Psi_2^{PBC}\right) = \left(\psi_{\alpha_1}, \psi_\beta\right)\left(\psi^{\alpha_1}, \psi^{\beta_1}\right)\left(\psi_{\alpha_2}, \psi_{\beta_1}\right) ... \\ ... \left(\psi_{\alpha_{N/2}}, \psi_{\beta_{(N-2)/2}}\right)\left(\psi^{\alpha_{N/2}}, \psi^\beta\right) = \delta_{\alpha_1\beta}\delta^{\alpha_1\beta_1} ... \delta^{\alpha_{N/2}\beta} = 2\end{aligned} \tag{4.21}$$

4.1.2.1. Diagrammatic Approach:

An alternative approach to these calculations can be done using the graphical representations introduced earlier. We can calculate the overlaps between states by the following algorithm:

1. Place the diagrams for the two states on top of each other;
2. Connect the corresponding sites with vertical lines (that represent the single site overlaps);
3. Each path in the graph corresponds to a Kronecker Delta between the beginning and the end indices (as can be easily seen by the explicit examples — (4.20) and (4.21));
4. A closed loop will contribute with a factor of — $\sum_\alpha \delta_{\alpha\alpha} = 2$.

The calculations (4.20) and (4.21) are done diagrammatically in [Figure 4.2.].

The graphical formalism can also be used to calculate the average of a local operator (e.g. S_i^a with $a = x, y, z$). The nontrivial action of S_i^a only happens in the i-th index, giving:

- $\left[S_i^a\psi\right]_\alpha = \frac{1}{2}\left[\sigma^a\right]_\alpha^{\ \beta}\psi_\beta$, for case of lower indices (covariant);
- $\left[S_i^a\psi\right]^\alpha = -\frac{1}{2}\epsilon^{\alpha\gamma}\left[\sigma^a\right]_\gamma^{\ \beta}\epsilon_{\beta\mu}\epsilon^{\mu\delta}\psi_\delta = -\frac{1}{2}\epsilon^{\alpha\gamma}\left[\sigma^a\right]_\gamma^{\ \beta}\epsilon_{\beta\mu}\psi^\mu$, for upper indices (contravariant)[7].

Where σ^a is a Pauli matrix. Graphically, we represent this action as **an operator insertion in the bond** next to the i-th site [Figure 4.2].

From these rules and [Figure 4.2 d)], we can conclude that the matrix element of S_i^a, for either Ψ_1^{PBC} or Ψ_2^{PBC}, is composed of a single diagram, whose value is zero:

$$\left(\Psi_{1,2}^{PBC}, S_i^a\Psi_{1,2}^{PBC}\right) = 2^{\frac{N-2}{2}-1}\left[\sigma^a\right]_\alpha^{\ \beta}\delta_\beta^{\ \alpha} = 2^{\frac{N}{2}-2}Tr\left[\sigma^a\right] = 0 \tag{4.22}$$

[6] Note that, for only two possible values for each index, the following result holds - $\sum_\alpha \epsilon_\alpha^\beta\epsilon_\gamma^\alpha = 0$, for all values of the free indices.

[7] Use was made of the result $\epsilon_{\alpha\beta}\epsilon^{\beta\gamma} = -\delta_\alpha^{\ \gamma}$.

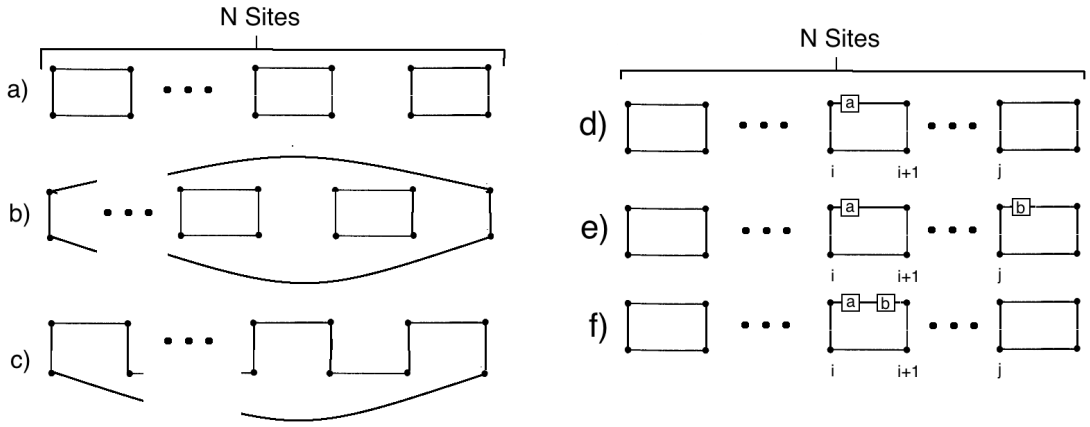


Figure 4.2.: **a**) - **c**) — Diagrammatic calculation of the norms and overlap between the two ground-states Ψ_1^{PBC} or Ψ_2^{PBC} . **d**) - **f**) — Some examples of diagrams associated, respectively with $(\Psi_1^{PBC}, S_i^a \Psi_1^{PBC})$, $(\Psi_1^{PBC}, S_i^a S_j^b \Psi_1^{PBC})$ for i and j not connected an also with $(\Psi_1^{PBC}, S_i^a S_{i+1}^b \Psi_1^{PBC})$ for neighbors in contracted into a singlet. The black boxes represent the insertion of Pauli matrices $[\sigma^a]_\alpha^\beta$. When there are two insertions in the same link, we have — $[\sigma^a]_\alpha^\beta \left[\sigma^b\right]_\gamma^\alpha \equiv [\sigma^a]_\alpha^\beta \epsilon^{\alpha\mu} \left[\sigma^b\right]_\mu^\delta \epsilon_{\delta\gamma}$.

4.1.2.2. Correlation Function and 'Spin-Peierls' Order

Furthermore, we also wish to calculate averages of the form $(\Psi_{1,2}^{PBC}, S_i^a S_j^b \Psi_{1,2}^{PBC})$ in the same way. We have two distinct cases:

1. If $|i-j| > 1$: Then the only diagram that contributes is the one in [Figure 4.2 e)], yielding the value:
$$2^{\frac{N}{2}-4} Tr\left[\sigma^a\right] Tr\left[\sigma^b\right] = 0$$

2. For the correlation function between nearest neighbors, we have two situations:
   a) The two neighbors are not connected by a bond: The diagram yields 0, again.
   b) They are connected by a bond: The corresponding diagram yields[8]:
$$-2^{\frac{N}{2}-2} Tr\left[\left[\sigma^a\right]_\alpha^\beta \epsilon^{\alpha\gamma} \left[\sigma^b\right]_\gamma^\delta \epsilon_{\delta\mu}\right] = -2^{\frac{N}{2}-1}\delta^{ab}$$

Since every two consecutive sites are connected by a bond in either Ψ_1^{PBC} or Ψ_2^{PBC}, one concludes the following:

$$(\Phi^\pm, S_i^a S_j^b \Phi^\pm) = \frac{1}{2}\left[(\Psi_1^{PBC}, S_i^a S_j^b \Psi_1^{PBC}) + (\Psi_2^{PBC}, S_i^a S_j^b \Psi_2^{PBC})\right] = \begin{cases} 0 & if \ \ |i-j| \geq 2 \\ -2^{\frac{N}{2}-2}\delta^{ab} & if \ \ |i-j| = 1 \end{cases} \tag{4.23}$$

[8] By a direct calculation, one sees that $\epsilon^{\alpha\gamma}\left[\sigma^a\right]_\gamma^\delta \epsilon_{\delta\mu} = \left[\sigma^a\right]_\delta^\alpha$, for each $a = x, y, z$. Therefore, the raising/lowering of both indices is irrelevant for the Pauli Matrices.

Meaning that the correlation function between spins is:

$$C^{(\pm)ab}(|i-j|) = \frac{(\Phi^{\pm}, S_i^a S_j^b \Phi^{\pm})}{(\Phi^{\pm}, \Phi^{\pm})} = \begin{cases} 0 & if \ \ |i-j| \geq 2 \\ -\frac{1}{4}\delta^{ab} & if \ \ |i-j| = 1 \end{cases} \tag{4.24}$$

The result (4.24) tell us two important things about the nature of the ground-states of this model:

1. First of all, there is **No Long-Range Magnetic Order**, since the correlation functions drop to zero already for second-neighbors.
2. Secondly, it exhibits a special kind of order called **Spin-Peierls Order,** where every spin is perfectly anti-correlated with its first-neighbors and uncorrelated with all the others.

4.1.3. Are the Dimerized States the only Ground-States?

References: [31,32]

Last section, we have assumed that the only ground-states of this model are the RVB states, and the proof of this fact will be given in this section. The result can be stated in the form of the following theorem:

Theorem 1 (Ground-States of the Majumdar-Ghosh Model):

Any ground-state — $\phi^{(N)}$ — of the Majumdar-Ghosh Model, in a chain with N spins can always be written as:

$$\phi^{(N)} = A\Psi_1^{(N)} + B^{\alpha}_{\beta}\Psi_2^{(N)}{}_{\alpha}^{\ \beta} \qquad for\ even\ N \tag{4.25}$$

$$\phi^{(N)} = A^{\alpha}\Psi_{1\,\alpha}^{(N)} + B^{\beta}\Psi_2^{(N)}{}_{\beta} \qquad for\ odd\ N \tag{4.26}$$

Where A, A^{α}, B^{β} and B^{α}_{β} are arbitrary complex numbers (apart from normalization constraints).

- **Proof of the Theorem 1:**

To prove this result, we will use **an induction procedure over the number of spins** in the lattice. First, we need to remember that the system's Hamiltonian can be written as a sum of non-negative 3-spin operators, as follows:

$$H_{MG}^{(1,N)} = \sum_{i=1}^{N-2} H_i \Longrightarrow H_{MG}^{(1,N+1)} = H_{MG}^{(1,N)} + H_{N-1} \tag{4.27}$$

Where $H_i = \frac{3J}{4} P_{3/2}(i, i+1, i+2)$[9]. To start the induction, we can see that it works for $N = 3$, where the dimension of the ground-state manifold is known to be 4 and (4.28) exhausts all the possibilities[10]:

$$\phi^{(3)} = A^{\alpha}\psi_{\alpha}\psi^{\beta}_{\ \beta} + B^{\gamma}\psi_{\delta}^{\ \delta}\psi_{\gamma} \tag{4.28}$$

Starting from the case $N = 3$, we can build an inductive procedure to prove the result for any chain size. We just have to impose that $\phi^{(N+1)}$ **must be a simultaneous ground-state of both** $H_{MG}^{(1,N)}$ **and** H_{N-1}**.** Then, we have two distinct cases to consider:

- For **even** N, we have (by hypothesis) that the N-chain's ground-state is:

$$\phi^{(N)} = A\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{N/2}}\psi^{\alpha_{N/2}} + B^{\alpha}_{\ \beta}\psi_{\alpha}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-2)/2}}\psi^{\alpha_{(N-2)/2}}\psi^{\beta} \tag{4.29}$$

Adding an extra spin, yields:

$$\Psi^{(N+1)} = A^{\gamma}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{N/2}}\psi^{\alpha_{N/2}}\psi_{\gamma} + B^{\alpha\ \gamma}_{\ \beta}\psi_{\alpha}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-2)/2}}\psi^{\alpha_{(N-2)/2}}\psi^{\beta}\psi_{\gamma} \tag{4.30}$$

However, not all the components in (4.30) keep the highest-spin projection null, for the last trio of spins. This means that they are excited states of H_{N-1}. By keeping only the allowed components, we get:

$$\begin{aligned}\phi^{(N+1)} &= A^{\gamma}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{N/2}}\psi^{\alpha_{N/2}}\psi_{\gamma} + B^{\alpha\ \beta}_{\ \beta}\psi_{\alpha}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-2)/2}}\psi^{\alpha_{(N-2)/2}}\psi^{\beta}\psi_{\beta} = \\ &= A^{\gamma}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{N/2}}\psi^{\alpha_{N/2}}\psi_{\gamma} + C^{\alpha}\psi_{\alpha}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-2)/2}}\psi^{\alpha_{(N-2)/2}}\psi^{\beta}\psi_{\beta}\end{aligned} \tag{4.31}$$

Which is the expected result.

- For **odd** N**,** we can do a similar reasoning, i.e.:

$$\phi^{(N)} = A^{\beta}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-1)/2}}\psi^{\alpha_{(N-1)/2}}\psi_{\beta} + B^{\alpha}\psi_{\alpha}\psi^{\alpha_1}\psi_{\alpha_1}...\psi^{\alpha_{(N-1)/2}}\psi_{\alpha_{(N-1)/2}} \tag{4.32}$$

Adding an extra spin yields (4.33):

$$\Psi^{(N+1)} = C^{\beta}_{\ \gamma}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-1)/2}}\psi^{\alpha_{(N-1)/2}}\psi_{\beta}\psi^{\gamma} + B^{\alpha}_{\ \beta}\psi_{\alpha}\psi^{\alpha_1}\psi_{\alpha_1}...\psi^{\alpha_{(N-1)/2}}\psi_{\alpha_{(N-1)/2}}\psi^{\beta} \tag{4.33}$$

While the condition that $\Psi^{(N+1)}$ must also be a ground-state of H_{N-1} demands that we only keep the terms in (4.34)

$$\begin{aligned}\phi^{(N+1)} &= C^{\beta}_{\ \beta}\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-1)/2}}\psi^{\alpha_{(N-1)/2}}\psi_{\beta}\psi^{\beta} + B^{\alpha}_{\ \beta}\psi_{\alpha}\psi^{\alpha_1}\psi_{\alpha_1}...\psi^{\alpha_{(N-1)/2}}\psi_{\alpha_{(N-1)/2}}\psi^{\beta} = \\ &= E\psi_{\alpha_1}\psi^{\alpha_1}...\psi_{\alpha_{(N-1)/2}}\psi^{\alpha_{(N-1)/2}}\psi_{\beta}\psi^{\beta} + B^{\alpha}_{\ \beta}\psi_{\alpha}\psi^{\alpha_1}\psi_{\alpha_1}...\psi^{\alpha_{(N-1)/2}}\psi_{\alpha_{(N-1)/2}}\psi^{\beta}\end{aligned} \tag{4.34}$$

[9]The Hamiltonian defined in (4.27) is just a shifted version of the Majumdar-Ghosh Hamiltonian (4.1), such that all eigenvalues are non-negative.

[10]Technically, the set of states $\left\{\psi_{\alpha}\psi^{\beta}_{\ \beta}, \psi_{\delta}^{\ \delta}\psi^{\gamma}\right\}$ is not orthonormal, however they are linearly independent, and that is enough for this argument to hold.

This proves the result for any Majumdar-Ghosh chain.

□

4.1.4. The Thermodynamic Limit of the Majumdar-Ghosh Model

References: [32]

In this subsection, we wish to explore the $N \to \infty$ limit of this model. For that, we will consider always chains with an odd length centered at zero — $\{$-L,$-L+1$, ... ,$L-1$,$L\}$ — for which the ground-states are fourfold degenerate and given in (4.26).

Naively, one would assume that taking the thermodynamic limit would preserve the dimension of the ground-state manifold, but it turns out to be much more subtle than that. The main reason for this has to do with the fact that **some of these states cannot be distinguished by any local measurement**. From a physical point of view, they have to be considered the same.

We intend to prove the following result:

Theorem 2 (Ground-States of the Infinite Majumdar-Ghosh Chain):

For any local observable A^a with support contained in $\{-L+2, \ldots, L-2\}$, the expectation value:

$$\omega_i(A) \equiv \frac{\left(\Psi_{i\ \ \alpha}^{(2L+1)}, A\Psi_{i\ \ \alpha}^{(2L+1)}\right)}{\left(\Psi_{i\ \ \alpha}^{(2L+1)}, \Psi_{i\ \ \alpha}^{(2L+1)}\right)} \quad ; \quad i = 1, 2 \tag{4.35}$$

is independent of L and α. This means that, after taking the limit $L \to \infty$, we will only observe the existence of a doubly-degenerate ground-state for this model.

[a] In this context, a local observable stands for an hermitian linear operator that acts non-trivially only for a finite number of tensor components of the many-body Hilbert Space - $\mathscr{H} = \otimes_{i \in \mathscr{L}} \mathscr{H}_i$

- **Proof of the Theorem 2:**

If we suppose that the support of A is inside $\{$-l,$-l+1$, ... ,$l-1$,$l\}$, for $l < L-1$, we need to prove that (4.35) is independent of L and α (but dependent of i) for at least one cleverly chosen local observable.

- **Independence in L and α:**

To prove **the independence on** L, one just has to realize that $\Psi_{i\ \ \alpha}^{(L)}$ are tensor product states, between pairs of spins (and an individual spin at one of the edges). This fact allows the following decomposition of the expectation value of A (for $i = 1$, since the other case is analogous):

$$\left(\Psi_{1\ \alpha}^{(2L+1)}, A\Psi_{1\ \alpha}^{(2L+1)}\right) = \left(\Psi_1^{(L-l)}, \Psi_1^{(L-l)}\right)\left(\Psi_{1\ \gamma}^{(2l+1)}, A\Psi_{1\ \gamma}^{(2l+1)}\right)\left(\Psi_{2\ \alpha}^{(L-l)\,\gamma}, \Psi_{2\ \alpha}^{(L-l)\,\gamma}\right) \tag{4.36}$$

This decomposition is depicted in the Figure 4.3. From the earlier results — (4.20) — we can see that:

1. The overlaps $\left(\Psi_1^{(L-l)}, \Psi_1^{(L-l)}\right)$ and $\left(\Psi_{2\ \alpha}^{(L-l)\,\gamma}, \Psi_{2\ \alpha}^{(L-l)\,\gamma}\right)$ are of the order $2^{L/2}$;
2. The norm $\left(\Psi_{i\ \alpha}^{(2L+1)}, \Psi_{i\ \alpha}^{(2L+1)}\right) \sim 2^L$;
3. Also, the average $\left(\Psi_{1\ \alpha}^{(2l+1)}, A\Psi_{1\ \gamma}^{(2l+1)}\right)$ is independent of L;

Therefore, we conclude that (4.35) is independent of L for a large enough chain.

On the other hand, **the independence on** α is clear from the fact that this free index is related only with an edge spin-state, outside the support of the A observable.

- **Distinguishability between the states** $i = 1, 2$ **:**

Finally, we must check that there is a local operator whose expectation value depends on $i = 1, 2$, distinguishing those two states, even in this limit. That operator can be chosen to be $B = -4S_1^z S_2^z$, which **yields zero in the case where the spins 1 and 2 are not-contracted** and **yields one if they belong to a singlet**. [11]

We conclude then, that the infinite Majumdar-Ghosh chain shares the same multiplicity of ground-states as the periodic chain, a fact that had already been pointed out. This completes the proof.

□

4.1.5. The Low-Energy Spectrum of the Model

References: [31,32]

Besides knowing the exact ground-states, we also which to characterize the low-energy excitations of this model. In fact, this was first attempted in one of the original papers by C. K. Majumdar [30], using an approximate approach similar to the usual Spin-Wave theory (Chapter 1).

In this article, he obtained a gapless spectrum with a linear dispersion relation (near the Γ-point), which would lead to the same kind of divergences that affect the 1-dimensional AFM spin-wave theory of the Heisenberg Model. Nevertheless, almost 20 years later, AKLT were able to prove in [32], that the spectrum of this model is actually gapped, invalidating these first results.

In this section, we will reproduce (with detail) the proof of [32] and show that there is indeed an energy gap above the ground-states. Mathematically, this result can be casted in the form of the following theorem:

[11] If we remember the construction of the states $\Psi_1^{(N)}$ and $\Psi_2^{(N)}$, it is obvious that B acts like a filter that distinguishes both states.

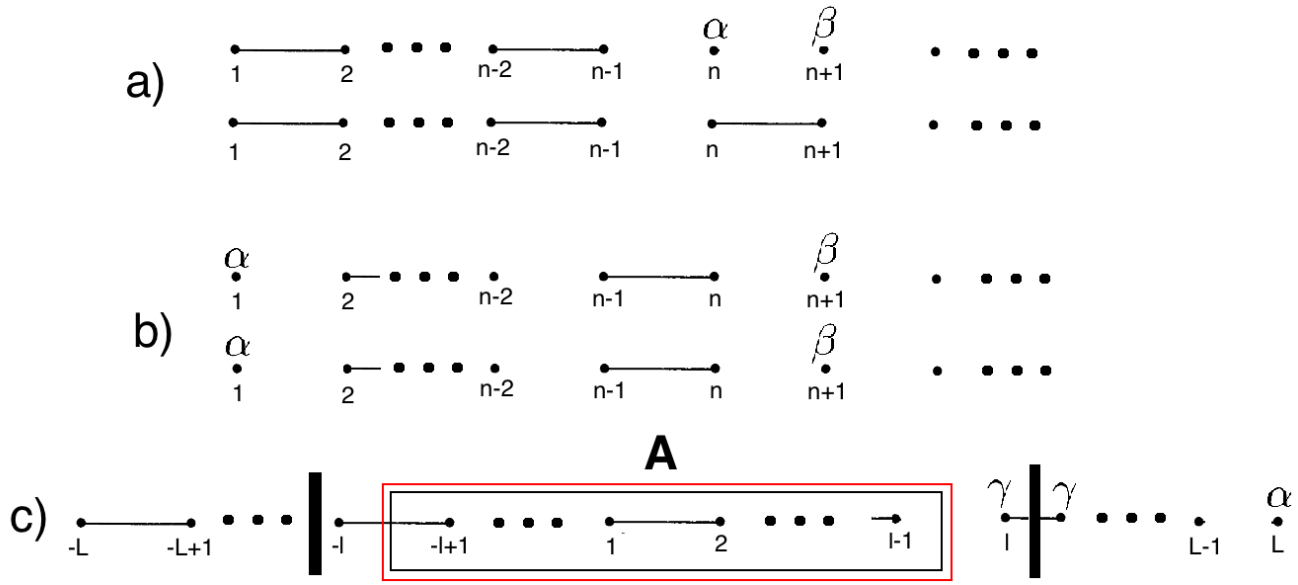


Figure 4.3.: **a)** and **b)** — Represent two examples, where we go from a ground-state of $H^{(1,n)}$ (on top) and the corresponding ground-state of $H^{(1,n+1)}$ (in the bottom). It is clear from the scheme that one loses 3 ground-states when an extra term is added to the Hamiltonian. **c)** — Represents a length $2L+1$ chain with a local operator A acting non-trivially only in its support (marked by a rectangle). The black bars represent the decomposition done in equation (4.36).

Theorem 3 (The Majumdar-Ghosh Model has a Gapped Spectrum)

For any state ψ which is orthogonal to any of the ground-states of the chain with length N, there is a positive number Δ (independent of N), such that:

$$\left(\psi, H_{MG}^{(1,N)}\psi\right) \geq \Delta\,(\psi,\psi) \tag{4.37}$$

- **Motivation for this proof:**

The main idea of this proof will be to consider the Hilbert space associated with a whole semi-infinite chain — $\mathscr{H} = \mathscr{H}_{site}^{\otimes\infty}$— and consider partial Hamiltonians that involve only interactions among a finite subset of those spins. Obviously, if an Hamiltonian H_1 contains another H_2 , then the ground-states of H_1 will be also ground-states of H_2, but the opposite is not true. Furthermore, if two Hamiltonians refer to non-intersecting sets of spins, they will commute and a set of common ground-states can be chosen.

Using these ideas, it will be possible obtain a bound for the finite chain Hamiltonian but before, we need to fix some notation and prove two auxiliary lemmas.

- **Conventions and Definitions:**

We begin by fixing the following notation:

- We will call $H_{MG}^{(i,j)} = \sum_{k=i}^{j-2} H_k$, the Hamiltonian that describes the mutual interactions connecting the sites from i to j in the chain;
- $Q_{i,j}$ will be the projector onto the states of $\mathscr{H}$ which are ground-states of $H_{MG}^{(i,j)}$,
- Q_n will represent the projector onto de ground-state manifold of $H_{MG}^{(1,n)}$;
- $P_n = \mathbb{I} - Q_n$ will be the complementary projector to Q_n.

As referred before, we know that **any ground-state of $H^{(1,n)}$ is also a ground-state of $H^{(1,m)}$, if** $m \leq n$. This means that the following inclusions are true (for the image subspaces):

$$Im[Q_n] \supseteq Im[Q_{n+1}] \Rightarrow Im[P_n] \subseteq Im[P_{n+1}] \tag{4.38}$$

It is also true that (for $l < N$):

$$P_N = P_N - P_{N-1} + P_{N-1} - ... + P_{l+l} - P_l + P_l = \sum_{k=l}^{N-1} (P_{k+1} - P_k) + P_l \tag{4.39}$$

The terms in the above sum — $P_{k+1} - P_k = Q_k - Q_{k+1}$ — are just projectors onto the the set of ground-states of $H^{(1,k)}$ that are not ground-states of $H^{(1,k+1)}$. This last equation is the basis for our proof, since we will be able to upper-bound the right-hand-side in terms of the finite chain Hamiltonian.

Also, since we know the dimension of the ground-state manifolds of each of the finite Hamiltonians, we can easily deduce that (See [Figure 4.3 a) and b] for a depiction of the case when k is even):

$$dim\left[Im\left[Q_k - Q_{k+1}\right]\right] = \begin{cases} 6 & if\ k\ is\ even \\ 3 & if\ k\ is\ odd \end{cases} \tag{4.40}$$

Finally, we designate the set $\{\varphi_k^i\}_i$ to be an orthonormal basis for the subspace $Im\left[Q_k - Q_{k+1}\right]$ and use it to define the following state(where $l < N$ is an arbitrary positive integer):

$$\psi_{n+1}^i \in \mathscr{H} \equiv \frac{Q_{n-l+1,n+1}\varphi_{n+1}^i}{\left\|Q_{n-l+1,n+1}\varphi_{n+1}^i\right\|} \tag{4.41}$$

And also the constant:

$$\varepsilon(l) \equiv \sup_n \max_i \left\|Q_{n-l+1,n+1}\varphi_{n+1}^i\right\|^2 \tag{4.42}$$

- **Auxiliary Lemmas:**

We will now prove two general results. First, we will prove a bound for each of the terms in the sum (4.39).

Lemma 1:

Let ϵ_{l+1} be the lowest positive eigenvalue of $H_{MG}^{(1,l+1)}$, then the following inequality holds[a]:

$$P_{n+1} - P_n = Q_n - Q_{n+1} \leq 3\varepsilon(l) \sum_{i=1}^{dim[Q_k - Q_{k+1}]} P(\psi_{n+1}^i) + \frac{3}{\epsilon_{l-1}} H_{MG}^{(n-l+1,n+1)} \tag{4.43}$$

Where $P(\psi_{n+1}^i)$ is the projector onto states of the form $\psi_{n+1}^i \otimes \chi_{n+1,N}$, for any state $\chi_{n+1,N}$. Note that the range of the summation in (4.43) will be different if n is odd or even.

[a] In the following context, an inequality between operators is meant to be understood as an inequality of the average values relative to any state in $\mathscr{H}$. I.e., if $A \geq B \Longrightarrow (\chi, A\chi) \geq (\chi, B\chi)$, for any $\chi \in \mathscr{H}$.

- **Proof of Lemma 1:**

We start by noticing the following (where $Q \equiv Q_{n-l+1,n+1}$):

$$\begin{aligned}
\left(\chi, P(\varphi_{n+1}^i)\chi\right) &= \left|\left(\chi, \varphi_{n+1}^i\right)\right|^2 = \left|\left(\chi, Q\varphi_{n+1}^i + (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right|^2 \leq \\
&\leq \left(\left|\left(\chi, Q\varphi_{n+1}^i\right)\right| + \left|\left(\chi, (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right|\right)^2 = \\
&= \left|\left(\chi, Q\varphi_{n+1}^i\right)\right|^2 + \left|\left(\chi, (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right|^2 + 2\left|\left(\chi, Q\varphi_{n+1}^i\right)\right|\left|\left(\chi, (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right| \leq \\
&\leq 3\left|\left(\chi, Q\varphi_{n+1}^i\right)\right|^2 + 3\left|\left(\chi, (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right|^2
\end{aligned} \tag{4.44}$$

Where it was used the fact that, for $a, b \geq 0$, one has $(a+b)^2 \leq 3a^2 + 3b^2$[12]. Now, the first term in (4.44) can be rewritten, by using the definitions of ψ_{n+1}^i and $\varepsilon(l)$ — (4.41) and (4.42). I.e.:

$$3\left|\left(\chi, Q\varphi_{n+1}^i\right)\right|^2 = 3\left\|Q\varphi_{n+1}^i\right\|^2 \left(\chi, P(\psi_{n+1}^i)\chi\right) \leq 3\varepsilon(l)\left(\chi, P(\psi_{n+1}^i)\chi\right) \tag{4.45}$$

Since φ_{n+1}^i is a basis state for $Im\left[Q_n - Q_{n+1}\right]$, we know that — $(\chi, [Q_n - Q_{n+1}]\,\chi) = \sum_i \left(\chi, P(\varphi_{n+1}^i)\chi\right)$ — and, then we can use (4.44) and (4.45) to write:

$$(\chi, [Q_n - Q_{n+1}]\,\chi) \leq 3\varepsilon(l)\sum_i \left(\chi, P(\psi_{n+1}^i)\chi\right) + 3\sum_i \left|\left(\chi, (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right|^2 \tag{4.46}$$

It remains only to deal with the last term in (4.46). For that, we just have to remember that $\{\varphi_{n+1}^i\}_i$ is an orthonormal set of vectors in $\mathscr{H}$, which means that:

$$\sum_i \left|\left(\chi, (\mathbb{I} - Q)\,\varphi_{n+1}^i\right)\right|^2 = \sum_i \left|\left(\varphi_{n+1}^i, (\mathbb{I} - Q)\,\chi\right)\right|^2 \leq \left\|(\mathbb{I} - Q)\,\chi\right\|^2 = (\chi, (\mathbb{I} - Q)\,\chi) \tag{4.47}$$

Then, (4.46) becomes:

[12] The proof of this is done by expanding $(a+b)^2 = a^2 + b^2 + 2ab$ and considering two cases: 1)$a \geq b$, then $(a+b)^2 \leq 3a^2 + b^2 \leq 3a^2 + 3b^2$; 2)$b \geq a$, then $(a+b)^2 \leq a^2 + 3b^2 \leq 3a^2 + 3b^2$.

$$(\chi, [Q_n - Q_{n+1}]\,\chi) \leq 3\varepsilon(l) \sum_i \left(\chi, P(\psi^i_{n+1})\chi\right) + 3\,(\chi, (\mathbb{I} - Q)\,\chi) \tag{4.48}$$

Finally, since $(\mathbb{I} - Q)$ is a projector onto the excited states of $H^{(n-l+1,n+1)}$, we have — $(\chi, (\mathbb{I} - Q)\,\chi) \leq \left(\chi, \frac{1}{\epsilon_{l+1}} H^{(n-l+1,n+1)}_{MG}\chi\right)$ — for any state $\chi \in \mathscr{H}$ (ϵ_{l+1} being the lowest non-zero eigenvalue[13] of $H^{(n-l+1,n+1)}_{MG}$).

Then, we get to the final result:

$$(\chi, [Q_n - Q_{n+1}]\,\chi) \leq 3\varepsilon(l) \sum_i \left(\chi, P(\psi^i_{n+1})\chi\right) + \frac{3}{\epsilon_{l+1}} \left(\chi, H^{(n-l+1,n+1)}_{MG}\chi\right) \tag{4.49}$$

□

The second important lemma goes as follows:

Lemma 2:

Let ψ^i_{n+1} and ψ^j_{m+1} be defined as in (4.41), such that $|m - n| > l$, then:

$$P(\psi^i_{n+1})P(\psi^j_{m+1}) = 0 \tag{4.50}$$

Where $P(\psi^i_{n+1})$ is the projector onto states of the form $\psi^i_{n+1} \otimes \chi_{n+1,N}$, for any state $\chi_{n+1,N}$, with the same definition for $P(\psi^j_{m+1})$.

Equation (4.50) is equivalent to the statement that the images of the corresponding projectors are orthogonal. This is expressed alternatively as (we have defined $Q^k \equiv Q_{k-l+1,k+1}$):

$$\left(\psi^i_{n+1} \otimes \chi_{n+2,N}, \psi^j_{m+1} \otimes \theta_{m+2,N}\right) = \left(Q^n\varphi^i_{n+1} \otimes \chi_{n+2,N}, Q^m\varphi^j_{m+1} \otimes \theta_{m+2,N}\right) = 0$$

Now, using the fact that — $[Q^n, Q^m] = 0$ for $m \geq n + l + 1$ — we can write the previous equation as follows:

$$\left(\psi^i_{n+1} \otimes \chi_{n+2,N}, \psi^j_{m+1} \otimes \theta_{m+2,N}\right) = \left(\varphi^i_{n+1} \otimes \chi_{n+2,N}, Q^m Q^n \varphi^j_{m+1} \otimes \theta_{m+2,N}\right) \tag{4.51}$$

In the proof that follows, we will **always assume that** $m > n + l$**,** with no loss of generality.

- **Proof of Lemma 2:**

[13] Note that $H^{(n-l+1,n+1)}_{MG}$ is a gapped Hamiltonian, since it involves only a finite number of spin degrees of freedom.

To prove the result, we start by noting that φ^j_{m+1} is a ground-state of $H^{(1,m)}_{MG}$ and also of $H^{(n-l+1,n+1)}_{MG}$, meaning that — $Q^n\varphi^j_{m+1} = \varphi^j_{m+1}$. Since Q^m only acts non-trivially on states between $m-l+1$ and $m+1$ (and $m-l+1 > n+1$), then $Q^m\varphi^j_{m+1}$ is still a ground-state of $H^{(1,n+1)}_{MG}$. But φ^i_{n+1} is also orthogonal to all the ground-states of $H^{(1,n+1)}_{MG}$, by definition. This demonstrates the orthogonality between φ^i_{n+1} and $Q^mQ^n\varphi^i_{n+1}$, thus proving the Lemma.

□

4.1.5.1. The Fundamental Inequality

At last, we can use the inequality (4.43), to upper-bound the sum $\sum_{n=l}^{N-1}(P_{n+1}-P_n)$ in (4.39).

In fact, one sees that the sum — $\sum_{n=l}^{N-1} H^{(n-l+1,n+1)}_{MG} = \sum_{i=1}^{N-l} H^{(i,l+i)}_{MG}$ — contains each one of the terms in the full chain Hamiltonian $H^{(1,N)}_{MG}$, at least once, and at most $l+1$ times. Therefore, we can establish the following:

$$\sum_{n=l}^{N-1} H^{(n-l+1,n+1)}_{MG} \leq (l+1)H^{(1,N)}_{MG} \tag{4.52}$$

Using (4.52) into (4.43), we get:

$$\sum_{n=l}^{N-1}(P_{n+1}-P_n) \leq 3\varepsilon(l)\sum_{n=l}^{N-1}\sum_{i=1}^{dim[Q_k-Q_{k+1}]} P(\psi^i_{n+1}) + \frac{3(l+1)}{\epsilon_{l-1}}H^{(1,N)}_{MG} \tag{4.53}$$

Finally, we just need to deal with the first term in the right-hand side, which is a sum of projectors. To do that, we notice that **Lemma 2** allows us to group the terms in the sum over n, into sets of mutually orthogonal projectors (which are bounded by the identity operator). All in all, we can form at most $l+1$[14] of those groups, getting the final result:

$$\sum_{n=l}^{N-1}(P_{n+1}-P_n) \leq 3(l+1)\max\{dim\,[Q_k-Q_{k+1}]\}\,\varepsilon(l) + \frac{3(l+1)}{\epsilon_{l-1}}H^{(1,N)}_{MG} \tag{4.54}$$

Finally, we can plug (4.54) in the expression (4.39), yielding:

$$P_N \leq 18(l+1)\varepsilon(l) + \frac{3(l+1)}{\epsilon_{l-1}}H^{(1,N)} + P_l \leq 18(l+1)\varepsilon(l) + \left(\frac{3(l+1)}{\epsilon_{l-1}} + \frac{1}{\epsilon_l}\right)H^{(1,N)}_{MG} \tag{4.55}$$

In (4.55), we used the fact that:

$$P_l \leq \frac{1}{\epsilon_l}H^{(1,l)}_{MG} \leq \frac{1}{\epsilon_l}H^{(1,L)}_{MG}$$

Which can be checked to be true for both ground-states and also excited states. From (4.55) we can draw the following rigorous inequality:

[14]It will be equal to this, if $N-1 > 2l$, otherwise it will certainly by less than that.

Lemma 3 (Fundamental Inequality for the MG Model):

For the Majumdar-Ghosh Model in a chain with N spins, the following inequality is true for any state ψ orthogonal to the ground-state manifold:

$$[1 - 18(l+1)\varepsilon_{MG}(l)]\,(\psi,\psi) \leq \left(\frac{3(l+1)}{\epsilon_{l-1}} + \frac{1}{\epsilon_l}\right)\left(\psi, H_{MG}^{(1,N)}\psi\right) \tag{4.56}$$

Where l is an arbitrary integer in $\{1, ..., N-1\}$, $\epsilon_l/\epsilon_{l+1}$ are the lowest non-zero eigenvalues of $H^{(1,l)}/H^{(1,l+1)}$ and $\varepsilon_{MG}(l) \equiv \sup_n \max_i \left\|Q_{n-l+1,n+1}\varphi_{n+1}^i\right\|^2$.

The similarity between (4.56) and the wanted result of the **Theorem 3** is staggering. However, (4.56) can only be reduced to that result if we are able to prove that there is an l such that:

$$1 - 18(l+1)\varepsilon_{MG}(l) > 0$$

This condition will be guaranteed by the following result:

Lemma 4 (The ε_{MG} bound):

There is a positive constant c such that, for every even integer l, we have the following inequality:

$$\varepsilon_{MG}(l) \equiv \sup_n \max_i \left\|Q_{n-l+1,n+1}\varphi_{n+1}^i\right\|^2 \leq c2^{-l/2} \tag{4.57}$$

This Lemma is proved by explicitly writing the conditions that define the state φ_{n+1}^i, when it is written in the basis of [Figure 4.4.] and seeing what will be the order of magnitude of the respective coefficients. The basis used to represent the state is chosen for convenience, since it will be easy to see the effect of $Q_{n-l+1,n+1}$ in each of these states.

Now, we will formalize these ideas. Once again, we will use the shortened notation — $Q = Q_{n-l+1,n+1}$.

- **Proof of Lemma 4:**

To do the proof, we start by writing a general expression for the states φ_{n+1}^i, assuming n to be odd. Using the basis of states defined in [Figure 4.4], we can immediately write (4.58), since we know φ_{n+1}^i is a ground-state of $H_{MG}^{(1,n)}$:

$$\varphi_{n+1}^i = A^{(i)\gamma}{}_{\delta}\psi^{(12)\,\alpha\,\delta}_{\alpha\,\gamma} + B^{(i)\gamma}{}_{\delta}\psi^{(21)\,\delta}_{\gamma} \tag{4.58}$$

However, the state (4.58) still needs to be normalized. That condition is expressed as follows:

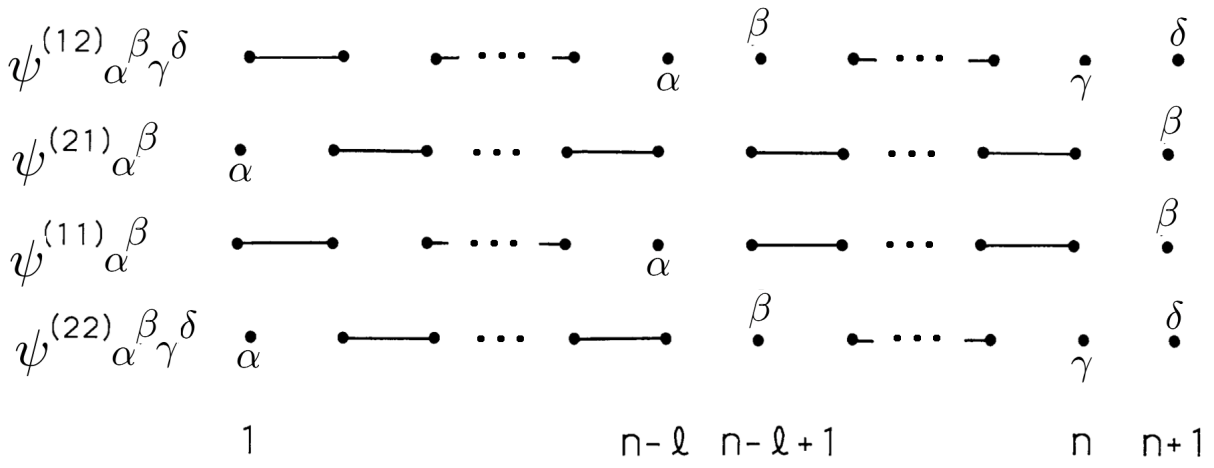


Figure 4.4.: Graphical Representation of the basis states that span the subspace of the simultaneous ground-states of $H_{MG}^{(1,n-l)}$ and $H_{MG}^{(n-l+1,n)}$.

$$\left(\varphi_{n+1}^{i},\varphi_{n+1}^{i}\right)=\left[A^{(i)\gamma}{}_{\delta}\right]^{*}A^{(i)\mu}{}_{\nu}\left(\psi^{(12)\,\alpha\,\delta}_{\ \ \alpha\,\gamma},\psi^{(12)\,\beta\,\nu}_{\ \ \beta\,\mu}\right)+\left[B^{(i)\gamma}{}_{\delta}\right]^{*}B^{(i)\mu}{}_{\nu}\left(\psi^{(21)}{}_{\gamma}^{\ \delta},\psi^{(21)}{}_{\mu}^{\ \nu}\right)+$$
$$+\left[A^{(i)\gamma}{}_{\delta}\right]^{*}B^{(i)\mu}{}_{\nu}\left(\psi^{(12)\,\alpha\,\delta}_{\ \ \alpha\,\gamma},\psi^{(21)\,\nu}_{\ \ \mu}\right)+c.c.=1$$

Diagrammatically, we know that the only overlaps in the last expression, that scale with n are the following norms:

$$\left(\psi^{(12)\,\alpha\,\delta}_{\ \ \alpha\,\gamma},\psi^{(12)\,\beta\,\nu}_{\ \ \beta\,\mu}\right)=\left(\psi^{(21)}{}_{\gamma}^{\ \delta},\psi^{(21)}{}_{\mu}^{\ \nu}\right)=\delta^{\delta\nu}\delta_{\gamma\mu}2^{\frac{n-1}{2}}$$

All the others will be of the order of unity or null — $\left(\psi^{(12)\,\alpha\,\delta}_{\ \ \alpha\,\gamma},\psi^{(21)\,\nu}_{\ \ \mu}\right)=\delta^{\delta\nu}\delta_{\gamma\mu}$. Hence:

$$\sum_{\gamma,\delta}\left\{2^{\frac{n-1}{2}}\left[\left|A^{(i)\gamma}{}_{\delta}\right|^{2}+\left|B^{(i)\gamma}{}_{\delta}\right|^{2}\right]+\left[A^{(i)\gamma}{}_{\delta}\right]^{*}B^{(i)\gamma}{}_{\delta}+\left[B^{(i)\gamma}{}_{\delta}\right]^{*}A^{(i)\gamma}{}_{\delta}\right\}=1 \tag{4.59}$$

The only way this equation can be true for all odd values of n, is if $\left|A^{(i)\mu}{}_{\nu}\right|,\left|B^{(i)\mu}{}_{\nu}\right|\lesssim 2^{-\frac{n}{4}}$, for all $\mu,\nu=1,2$.

On the other hand, we must also impose that φ_{n+1}^{i} is orthogonal to any ground-state of $H^{(1,n+1)}$, i.e.:

$$\left(\psi^{(12)\,\alpha\,\beta}_{\ \ \alpha\,\beta},\varphi_{n+1}^{i}\right)=2^{\frac{n-1}{2}}A^{(i)\gamma}{}_{\gamma}+B^{(i)\gamma}{}_{\gamma}=0 \tag{4.60}$$

$$\left(\psi^{(21)\,\beta}_{\ \ \alpha},\varphi_{n+1}^{i}\right)=A^{(i)}_{\ \alpha}{}^{\ \beta}+2^{\frac{n-1}{2}}B^{(i)}_{\ \alpha}{}^{\ \beta}=0\ ,\ for\ all\quad\alpha,\beta=1,2 \tag{4.61}$$

The two above equations allow us to write the following relations:

$$\frac{\left|B^{(i)\gamma}{}_{\gamma}\right|}{\left|A^{(i)\gamma}{}_{\gamma}\right|}=2^{\frac{n-1}{2}}\ ;\quad\frac{\left|B^{(i)}_{\ \alpha}{}^{\ \beta}\right|}{\left|A^{(i)}_{\ \alpha}{}^{\ \beta}\right|}=2^{-\frac{n-1}{2}}\ ,\ for\ all\quad\alpha,\beta=1,2 \tag{4.62}$$

From these, we see that the bounds imposed by normalization can be further reduced, by imposing the orthogonality condition. The new bounds are:

$$\left|B^{(i)}{}_{\alpha}^{\ \beta}\right| \lesssim 2^{-\frac{3n}{4}} \quad ; \quad \left|A^{(i)}{}_{\alpha}^{\ \alpha}\right| \lesssim 2^{-\frac{5n}{4}}. \tag{4.63}$$

These inequalities can now be used to prove that $\left\|Q_{n-l+1,n+1}\varphi^i_{n+1}\right\| \lesssim 2^{-l/2}$. This is done in three steps:

- First, we use the **Triangle Inequality** to write:

$$\begin{aligned}\left\|Q\varphi^i_{n+1}\right\| &= \left\|A^{(i)\gamma}{}_{\delta}Q\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta} + B^{(i)\gamma}{}_{\delta}Q\psi^{(21)}{}_{\gamma}^{\ \delta}\right\| \leq \\ &\leq \left\|A^{(i)\gamma}{}_{\delta}Q\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}\right\| + \left\|B^{(i)\gamma}{}_{\delta}Q\psi^{(21)}{}_{\gamma}^{\ \delta}\right\|\end{aligned} \tag{4.64}$$

- The second term already obeys the wanted inequality, because Q is a projector (averages are between 0 and 1). This means that:

$$\left\|B^{(i)\gamma}{}_{\delta}Q\psi^{(21)}{}_{\gamma}^{\ \delta}\right\| \leq \left\|B^{(i)\gamma}{}_{\delta}\psi^{(21)}{}_{\gamma}^{\ \delta}\right\| \lesssim 2^{-\frac{3n}{4}} \times 2^{\frac{n}{4}} \lesssim 2^{-\frac{l}{2}} \quad for \quad any \quad l < n. \tag{4.65}$$

- Finally, it remains to be proven that $\left\|A^{(i)\gamma}{}_{\delta}Q\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}\right\| \lesssim 2^{-\frac{l}{2}}$. This norm can be written as:

$$\left\|A^{(i)\gamma}{}_{\delta}Q\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}\right\|^2 = \left(A^{(i)\gamma}{}_{\delta}Q\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}, A^{(i)\gamma}{}_{\delta}Q\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}\right) = A^{(i)\gamma}{}_{\delta}\left(\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}, Q\varphi'\right) \tag{4.66}$$

For $\varphi' = A^{(i)\gamma}{}_{\delta}\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}$. All we have to do is calculate the overlap between $Q\varphi'$ and the $\psi^{(12)}$ basis state. Recalling that $Q\varphi'$ is a ground-state of $H^{(n-l+1,n+1)}$ and also of $H^{(1,n-l)}$[15], it can be written as a linear combination of all the states in [Figure 4.4.].

$$Q\varphi' = C^{1}{}_{\beta}^{\ \alpha}\psi^{(11)}{}_{\alpha}^{\ \beta} + C^{2}{}_{\beta}^{\ \alpha}\psi^{(22)}{}_{\alpha\,\gamma}^{\beta\,\gamma} + C^{3}{}_{\beta}^{\ \alpha}\psi^{(21)}{}_{\alpha}^{\ \beta} + C^{4}{}_{\beta}^{\ \alpha}\psi^{(12)}{}_{\alpha\,\gamma}^{\beta\,\gamma} \tag{4.67}$$

For the same reasons as before, all the coefficients need to be of order less than $2^{-\frac{n}{4}}$, if the norm of (4.66) is to be under control. Using this last expression, one sees that we have to deal with 4 terms, as listed below:

$$C^{1}{}_{\beta}^{\ \alpha}A^{(i)\gamma}{}_{\delta}\left(\psi^{(12)}{}_{\mu\,\gamma}^{\mu\,\delta}, \psi^{(11)}{}_{\alpha}^{\ \beta}\right) = 2^{\frac{n-l-1}{2}}C^{1}{}_{\beta}^{\ \alpha}A^{(i)\gamma}{}_{\delta}\delta^{\beta\delta}\delta_{\gamma\alpha} \lesssim 2^{-\frac{l}{2}} \tag{4.68}$$

$$C^{2}{}_{\beta}^{\ \alpha}A^{(i)\gamma}{}_{\delta}\left(\psi^{(12)}{}_{\mu\,\gamma}^{\mu\,\delta}, \psi^{(22)}{}_{\alpha\,\nu}^{\beta\,\nu}\right) = 2^{\frac{l-1}{2}}C^{2}{}_{\beta}^{\ \alpha}A^{(i)\gamma}{}_{\delta}\delta_{\alpha}^{\beta}\delta_{\gamma}^{\delta} = 2^{\frac{l-1}{2}}C^{2}{}_{\alpha}^{\ \alpha}A^{(i)\gamma}{}_{\gamma} \lesssim 2^{\frac{l-3n-1}{2}} \lesssim 2^{-l} \tag{4.69}$$

$$C^{3}{}_{\beta}^{\ \alpha}A^{(i)\gamma}{}_{\delta}\left(\psi^{(12)}{}_{\mu\,\gamma}^{\mu\,\delta}, \psi^{(21)}{}_{\alpha}^{\ \beta}\right) = C^{3}{}_{\beta}^{\ \alpha}A^{(i)\gamma}{}_{\delta}\delta^{\beta\delta}\delta_{\gamma\alpha} \lesssim 2^{-\frac{n}{2}} \lesssim 2^{-\frac{l}{2}} \tag{4.70}$$

[15] This last fact is a consequence of the fact that $\left[H^{(1,n-l)}, Q\right] = 0$ and also the fact that $\psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta}$ is also a ground-state of $H^{(1,n-l)}$.

$$C_{\beta}^{4\,\alpha} A^{(i)\gamma}{}_{\delta} \left(\psi^{(12)}{}_{\mu\,\gamma}^{\mu\,\delta}, \psi^{(12)}{}_{\alpha\,\nu}^{\beta\,\nu} \right) = 2^{\frac{n-3}{2}} C_{\beta}^{4\,\alpha} A^{(i)\gamma}{}_{\delta} \delta_{\alpha}^{\beta} \delta_{\gamma}^{\delta} = 2^{\frac{n-3}{2}} C_{\alpha}^{4\,\alpha} A^{(i)\gamma}{}_{\gamma} \lesssim 2^{-n-\frac{3}{2}} \lesssim 2^{-l} \tag{4.71}$$

At last, it is clear that $\left\| A^{(i)\gamma}{}_{\delta} Q \psi^{(12)}{}_{\alpha\,\gamma}^{\alpha\,\delta} \right\| \lesssim 2^{-\frac{l}{4}}$ and putting everything together, we get:

$$\left\| Q\varphi_{n+1}^{i} \right\| \lesssim 2^{-\frac{l}{4}} \Rightarrow \varepsilon(l) \lesssim 2^{-\frac{l}{2}} \tag{4.72}$$

□

- **Proof of Theorem 3:**

At last, **Lemma 4** guarantees that, for a large enough value l_c, we can have $18(l_c+1)\varepsilon_{MG}(l_c) < 1$, which turns the inequality (4.56) into:

$$\Delta_{MG}(\psi, \psi) \leq \left(\psi, H_{MG}^{(1,N)} \psi \right) \tag{4.73}$$

With the definition:

$$\Delta_{MG} \equiv \left[\frac{1 - 18(l_c+1)\varepsilon_{MG}(l_c)}{\left(\frac{3(l_c+1)}{\epsilon_{l_c-1}} + \frac{1}{\epsilon_{l_c}} \right)} \right] > 0$$

Thus proving that there is a gap in the spectrum.

4.2. The One-Dimensional AKLT Model

References: [7,31,32]

In this section, we will use the tools and definitions of last section to build and explore a very special quantum antiferromagnetic model, in a chain of localized spin-1 degrees of freedom. This model was first described on 1987 by I. Affleck, T. Kennedy, E. Lieb and H. Tasaki [31,32], becoming a very important problem in the subject due to the mathematical techniques involved in its construction (and solution), but also because of the interesting properties of its ground-state.

The Hamiltonian of this model (in a finite chain with N spins) can be presented as:

$$H_{AKLT}^{N} = J \sum_{i=1}^{N-1} \left[\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + 1/3 \left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} \right)^2 \right] \tag{4.74}$$

Where $J > 0$ and $\overrightarrow{\mathbf{S}}_i$ are local spin-1 operators.

If one assumes the periodic boundary condition (PBC) — $\overrightarrow{\mathbf{S}}_{N+1} = \overrightarrow{\mathbf{S}}_1$ — we can write (4.73) as:

$$H_{AKLT}^{N,\,PBC} = J \sum_{i=1}^{N} \left[\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + 1/3 \left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} \right)^2 \right] \tag{4.75}$$

It is worth noticing that this model can be seen as an altered version of the spin-1 Heisenberg model since the interactions are still between nearest-neighbors. In fact, the extra term in the Hamiltonian does not create any classical frustration, as happened in the Majumdar-Ghosh case.

4.2.1. Building the Ground-State

To obtain the exact ground-state of this model, we proceed in a similar path as the one taken for the Majumdar-Ghosh case. We start by writing (4.73) and (4.74) as a sum of spin projectors for each pair of consecutive spins.

The Hilbert space for the whole lattice is, again — $\mathscr{H} = \otimes_{i=1}^{N} \mathscr{H}_i^{(s=1)}$. If we consider two consecutive spins, the Addition Theorem of Angular Momentum allow the following decomposition:

$$\mathscr{H}_i^{(s=1)} \otimes \mathscr{H}_{i+1}^{(s=1)} = 0 \oplus 1 \oplus 2$$

We can also write the expression for the projector onto the subspace with $j = 2$[16]:

$$\begin{aligned} P_2(i,i+1) &= \frac{1}{24} S_{Tot}^2 \left(S_{Tot}^2 - 2\right) = \frac{1}{6}\left(2 + \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right)\left(1 + \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right) = \\ &= \frac{1}{2}\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + \frac{1}{6}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right)^2 + \frac{1}{3} \end{aligned} \tag{4.76}$$

Using the last expression, we are able to write (4.73) as:

$$H_{AKLT}^N = 2J \sum_{i=1}^{N-1} P_2(i,i+1) - \frac{2J\,(N-1)}{3} \tag{4.77}$$

Looking at (4.76), we can see a striking parallel between this and the previous model. Apart from irrelevant constants, they both can be seen as sums of projectors onto the highest spin multiplet, for a set of consecutive spins (a trio in the MG case and a pair in the AKLT).

Hence, the problem of building a ground-state for (4.74) amounts to building a wavefunction that has a null spin-2 projection for every pair of neighboring spins, along the chain. To do that, we can imagine that instead of a spin-1 in each lattice site, one has a pair of spins-1/2, as is shown in [Figure 4.5 a)].

However, one needs to be careful not to introduce artificial degrees of freedom in the system (namely, local spin singlet states). To avoid this, we will take the states allowed at each site to be of the form:

$$\psi_{\alpha\beta}^{(i)} \equiv \frac{1}{\sqrt{2}}\left[\psi_\alpha \psi_\beta + \psi_\alpha \psi_\beta\right] \tag{4.78}$$

Where ψ_α represent the same states as in the last section. Since all the states in (4.77) belong to the triplet subspace of the two virtual spins in site i, by using them as a local basis, we guarantee that no

[16] This can be seen directly, since $S_{Tot}^2 |0,0\rangle = 0$, $\left[S_{Tot}^2 - 2\right]|1,m\rangle = 0$ and $S_{Tot}^2\left[S_{Tot}^2 - 2\right]|2,m\rangle = 24\,|2,m\rangle$.

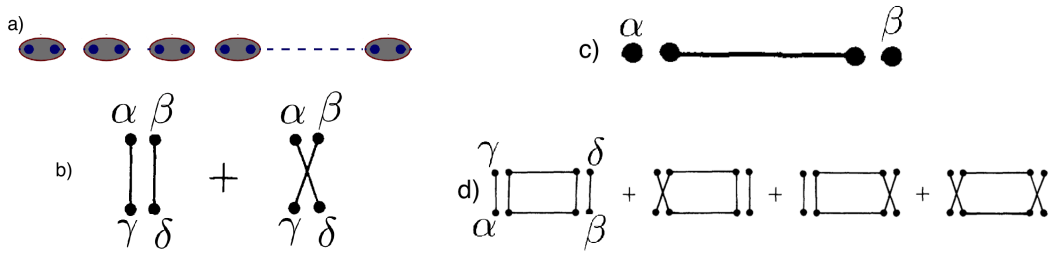


Figure 4.5.: **a)** The AKLT chain with the physical localized spins-1 replaced by pairs of virtual spins-1/2. **b)** The two diagrams that represent the overlap $(\psi_{\alpha\beta}, \psi_{\gamma\delta})$. **c)** Graphical representation of the ground-state for a pair of spins — $\Omega_\alpha^\gamma = \psi_{\alpha\beta}\psi^{\beta\gamma}$. **d)** Representation of the overlap — $\left(\Omega_\alpha^\beta, \Omega_\gamma^\delta\right)$ — in terms of diagrams.

artificial states are introduced in our construction. The overlaps between the states (4.77) can also be calculated using the definitions (4.18):

$$(\psi_{\alpha\beta}, \psi_{\gamma\delta}) = \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma} \tag{4.79}$$

The overlap in (4.78) can be expressed (in the diagrammatic language of last section), as the sum of two diagrams [Figure 4.5 b)].

As before, we can also define the upper-index version of the symmetric states — $\psi_{\alpha\beta}$:

$$\psi^{(i)\alpha\beta} = \epsilon^{\alpha\gamma}\epsilon^{\beta\delta}\psi^{(i)}_{\gamma\delta} \tag{4.80}$$

With the respective overlaps being given by:

$$\begin{aligned}\left(\psi^{\alpha\beta}, \psi^{\gamma\delta}\right) &= \epsilon^{\alpha\mu}\epsilon^{\beta\nu}\epsilon^{\gamma\rho}\epsilon^{\delta\sigma}\left(\psi_{\mu\nu}, \psi_{\rho\sigma}\right) = \delta^{\alpha\gamma}\delta^{\beta\delta} + \delta^{\alpha\delta}\delta^{\beta\gamma} \\ \left(\psi^{\alpha\beta}, \psi_{\gamma\delta}\right) &= \epsilon^{\alpha\mu}\epsilon^{\beta\nu}\left(\psi_{\mu\nu}, \psi_{\gamma\delta}\right) = \epsilon^{\alpha\gamma}\epsilon^{\beta\delta} + \epsilon^{\alpha\delta}\epsilon^{\beta\gamma}\end{aligned} \tag{4.81}$$

To build the AKLT ground-state, we start by focusing our attention at a given pair of neighboring spins of the lattice (which are to be seen as 4 spins-1/2, as shown in [Figure 4.5]). The Hilbert Space of those 4 virtual spins is 16-dimensional and can be decomposed as:

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 0 \oplus 1 \oplus 1 \oplus 2$$

A simple way to ensure that our state is orthogonal to the spin-2 subspace in the pair $(i, i+1)$ is to impose that one of the virtual spins in i is in a singlet state with one in $i+1$. This corresponds to contracting one of the indices of the local state in site i with one the site $i+1$, using the anti-symmetrical symbol. This procedure yields the following 4 states, for a single bond:

$$\Omega_\alpha^\gamma = \psi_{\alpha\beta}\psi^{\beta\gamma}\ ; \quad \alpha, \gamma = 1, 2 \tag{4.82}$$

The states (4.81) are also the only states of two spins that have the property of being orthogonal to the spin-2 multiplet, which can be proven by a simple counting argument[17].

This construction can be trivially generalized for the whole lattice. All the different cases are listed below:

- For an open chain with an even number of spins:

$$\Omega^{(N)}{}_{\alpha}^{\beta} = \psi_{\alpha\alpha_1}\psi^{\alpha_1\alpha_2}...\psi_{\alpha_{N-1}\alpha_N}\psi^{\alpha_N\beta} \tag{4.83}$$

- For an open chain with an odd number of spins:

$$\Omega^{(N)}_{\alpha\beta} = \psi_{\alpha\alpha_1}\psi^{\alpha_1\alpha_2}...\psi_{\alpha_N\alpha_{N-1}}\psi^{\alpha_{N-1}\alpha_N}\psi_{\alpha_N\beta} \tag{4.84}$$

- For a periodic chain:

$$\Omega^{(N)}_{PBC} = \Omega^{(N)}{}_{\alpha}^{\alpha} = \psi_{\alpha\alpha_1}\psi^{\alpha_1\alpha_2}...\psi_{\alpha_{N-1}\alpha_N}\psi^{\alpha_N\alpha} \tag{4.85}$$

In conclusion, the ground-states obtained in this way are essentially the same for N even or odd, and reduce to a single state, after imposing periodic boundary conditions.

The quantum manybody states (4.82)-(4.84) came to be known as **Valence-Bond Solid** (VBS) states, since they appear as a sequence of singlet contractions (Like the valence-bonds in Chemistry), but arranged in a way that mimics perfectly the underlying lattice. In other words, this construction does not break the lattice translational symmetry.

4.2.2. The AKLT States in the Product Basis

It is also possible to describe the VBS states, in terms of the standard product basis for $\mathscr{H}$ (as was easily done in the case if the MG model). To do that, we start by noticing two things:

- First of all, any product state can be uniquely defined by a string of +, - and 0's. Using the index notation, we have, for example[18]:

$$\begin{aligned}|00++00-0+...\rangle &= \frac{1}{2^{m/2}}\psi_{12}\psi_{12}\psi_{11}\psi_{11}\psi_{12}\psi_{12}\psi_{22}\psi_{12}\psi_{11}... = \\ &= (-1)^k\frac{1}{2^{m/2}}\psi_{12}\psi^{12}\psi_{11}\psi^{22}\psi_{12}\psi^{12}\psi_{22}\psi^{12}\psi_{11}\end{aligned}$$

Where m represents the number of +'s or -'s in the corresponding string and k is the number of 0's placed in even sites (counting from the left edge).

- Using the last identification, it is clear that (4.82)-(4.84) can be written as a linear combination of product states **represented only by strings which have alternation between + and -** (with as many zeros in between as we want).[19]

[17] This is seen just by noticing that the dimension of the subspace orthogonal to to the *spin*-2 is precisely 4. Since the 4 states in (4.81) are linearly independent, the former conclusion is trivial.
Linear independence follows from the fact that $\left(\Omega_{\alpha}^{\beta}, \Omega_{\gamma}^{\delta}\right) = \delta_{\alpha}^{\ \beta}\delta_{\gamma}^{\delta} + 3\delta_{\alpha\gamma}\delta_{\beta\delta}$, which indicates that only two of these states are non-orthogonal, but they are not proportional either.

[18] For that, we just have to notice that, by definition, one has $\psi_{11} = \sqrt{2}\,|+\rangle$, $\psi_{22} = \sqrt{2}\,|-\rangle$ and $\psi_{12} = \psi_{21} = |0\rangle$. Or, we can also use the overlaps (4.80), to prove that $\psi^{11} = \psi_{22} = \sqrt{2}\,|-\rangle$, $\psi^{22} = \psi_{11} = \sqrt{2}\,|+\rangle$ and $\psi^{12} = -\psi_{21} = -\,|0\rangle$.

[19] This can be seen easily by following up the values of the indices in the definitions (4.82)-(4.84). Furthermore, in the case of the open chain, the values of the edge indices fix if the allowed strings start by + or - (except for the case where there are only 0's, that is always allowed).

- The coefficients of the expansion will be reals with an absolute value of the form $2^{\#pairs\,(+,-)}$ and with a sign determined by the number of even sites holding 0's.

As an example, we can write one of the AKLT states for a chain of 4 spins:

$$\begin{aligned}\Omega^{(4)}{}_1{}^1 = &-|0000\rangle - 2\,|+-00\rangle - 2\,|0+-0\rangle + 2\,|+0-0\rangle - \\ &- 2\,|00+-\rangle + 2\,|0+0-\rangle - 2\,|+00-\rangle + 4\,|+-+-\rangle\end{aligned}$$

After the proper normalization, we get:

$$\begin{aligned}\Psi^{(4)}_{AKLT} = &\frac{4}{\sqrt{41}}\,|+-+-\rangle - \frac{1}{\sqrt{41}}\,|0000\rangle - \frac{2}{\sqrt{41}}\,|+-00\rangle - \frac{2}{\sqrt{41}}\,|0+-0\rangle + \\ &+ \frac{2}{\sqrt{41}}\,|+0-0\rangle - \frac{2}{\sqrt{41}}\,|00+-\rangle + \frac{2}{\sqrt{41}}\,|0+0-\rangle - \frac{2}{\sqrt{41}}\,|+00-\rangle\end{aligned}$$

And with this last expression, one can finally appreciate the amazing complexity of the AKLT state, which is very far from being a product state.

4.2.3. Order and Correlations in the AKLT Ground-States

Once again, the sets of states defined in (4.82)-(4.84) are not orthonormal, so it is important for us to calculate the norms and overlaps between all of them. This can be done diagrammatically, with the rules of last section, but remembering that now we will have an enormous amount of different diagrams contributing to each inner product. All the contributions must be summed over, in the end.

These calculations are done in the [Appendix D.1], the results being:

$$\left(\Omega^{(N)}{}_\alpha{}^\beta, \Omega^{(N)}{}_\gamma{}^\delta\right) = \delta_\alpha^\beta \delta_\gamma^\delta + \frac{1}{2}\left[3^N - 1\right]\delta_{\alpha\gamma}\delta^{\beta\delta}\ for\ N\ even \tag{4.86}$$

$$\left(\Omega^{(N)}_{\alpha\beta}, \Omega^{(N)}_{\gamma\delta}\right) = \delta_{\alpha\delta}\delta_{\beta\gamma} + \frac{1}{2}\left[3^N - 1\right]\delta_{\alpha\gamma}\delta^{\beta\delta}\ for\ N\ odd \tag{4.87}$$

Similarly to the Majumdar-Ghosh ground-states, the norms scale exponentially with N, while the overlaps between different states are either zero or of order 1. Also, from (4.85), we can easily obtain the norm of the only ground-state for the AKLT periodic chain:

$$\left(\Omega^{(N)}_{PBC}, \Omega^{(N)}_{PBC}\right) = \sum_{\alpha\gamma}\left(\Omega^{(N)}{}_\alpha{}^\alpha, \Omega^{(N)}{}_\gamma{}^\gamma\right) = 3^N + 3 \tag{4.88}$$

On the other hand, to calculate averages of observables in one of the AKLT ground-states, we will need to express the action of a local spin operator in the representation — $\psi_{\alpha\beta}$. That is easy, because the

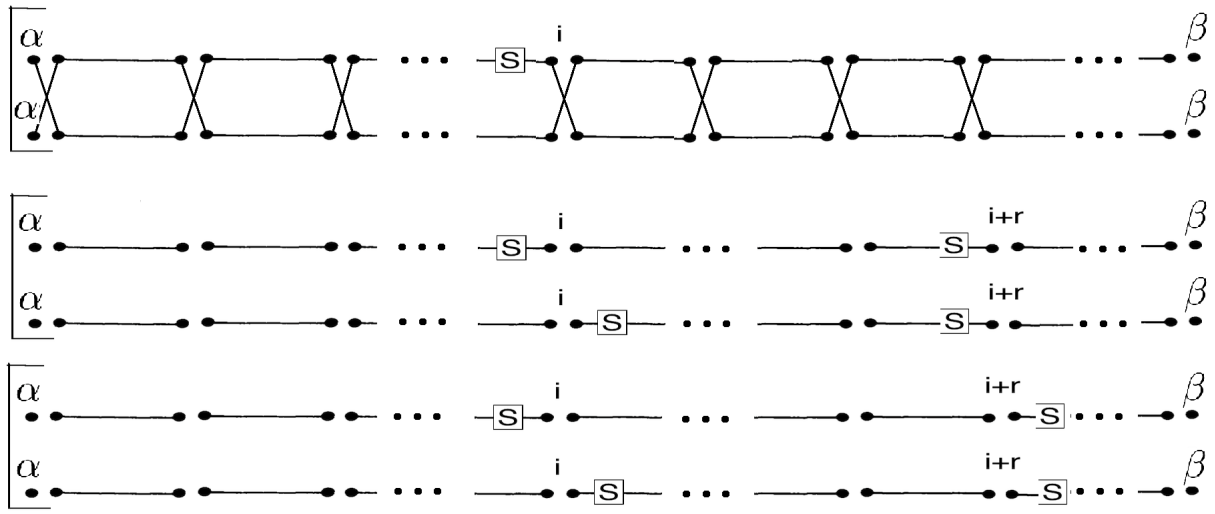


Figure 4.6.: **a)** Graphical Representation of the two terms in $S_i^a \Omega_{\alpha\beta}^{(N)}$. **b)** Representation of the 4 terms in $S_i^a S_{i+r}^b \Omega_{\alpha\beta}^{(N)}$.

spin one operator can be written as the sum of two spin-1/2 operators acting independently on each of the virtual spins. I.e.:

$$[S^a \psi]_{\alpha\beta} = 1/2 \left[\sigma^a{}_\alpha{}^\gamma \psi_{\gamma\beta} + \sigma^a{}_\beta{}^\gamma \psi_{\alpha\gamma} \right] \tag{4.89}$$

$$[S^a \psi]^{\alpha\beta} = -1/2 \left[\epsilon^{\alpha\mu} \sigma^a{}_\mu{}^\nu \epsilon_{\nu\gamma} \psi^{\gamma\beta} + \epsilon^{\beta\mu} \sigma^a{}_\mu{}^\nu \epsilon_{\nu\gamma} \psi^{\alpha\gamma} \right] \tag{4.90}$$

Where (4.88) represents the action on an **odd site** and (4.89) refers to the **even site**.

We know that $\epsilon^{\alpha\mu} \sigma^a{}_\mu{}^\nu \epsilon_{\nu\gamma}$ have exactly the same matrix elements as the original Pauli matrices $\sigma^a{}_\mu{}^\nu$, for all $a = x, y, z$ [footnote 7]. Therefore, we can interpret the action of S_i^a on a state, as breaking inserting a Pauli operator — $\pm 1/2 \sigma^a{}_\alpha{}^\gamma$ — in the link at the right or left of the site i (summing over the two cases in the end).

In the [Figure 4.6], we have represented two important cases - $S_i^a \Omega_{\alpha\beta}^{(N)}$ and $S_i^a S_{i+r}^b \Omega_{\alpha\beta}^{(N)}$.

Using the diagrammatic techniques developed for the MG model [Appendix D.2], we can calculate both the average local magnetization and the spin-spin correlation function in the AKLT states. In the limit of infinite volume, all of the states for the finite chain yield the same following results:

$$\left\langle \overrightarrow{\mathbf{S}}_i \right\rangle_{AKLT}^{\infty} = \lim_{N\to\infty} \left\{ \frac{\left(\Omega_{\alpha\beta}^{(N)}, \overrightarrow{\mathbf{S}}_i \Omega_{\alpha\beta}^{(N)} \right)}{\left(\Omega_{\alpha\beta}^{(N)}, \Omega_{\alpha\beta}^{(N)} \right)} \right\} = 0 \tag{4.91}$$

$$C^{ab}(r) = \lim_{N\to\infty} \left\{ \frac{\left(\Omega_{\alpha\beta}^{(N)}, S_i^a S_{i+r}^b \Omega_{\alpha\beta}^{(N)} \right)}{\left(\Omega_{\alpha\beta}^{(N)}, \Omega_{\alpha\beta}^{(N)} \right)} \right\} = 4/3 (-1)^r \delta^{ab} 3^{-r} = 4/3 (-1)^r \delta^{ab} e^{-r \ln 3} \tag{4.92}$$

From (4.91), we conclude that the system does not exhibit long-range AFM order, since the spin correlations decay exponentially with distance. The correlation length of the AKLT state is a little bit under one lattice spacing:

$$\xi_{AKLT} = \frac{1}{\ln 3} \simeq 0.910239$$

4.2.4. The Thermodynamic Limit of the AKLT Model

In the last section, we have found out that exact ground-states for the AKLT model can be obtained using the VBS construction, yielding a four-fold degenerate ground-state manifold in the finite chain case. However, we have observed that when PBC are imposed, only a single VBS ground-state emerges.

Furthermore, the calculation of the spin-spin correlations have given identical results for all of the 4 original ground-state, in the limit of an infinite chain, In this section, we will understand that such behavior is merely indicative that, in the thermodynamic limit, no local observable allows for the distinction between the 4 states $\Omega_{\alpha\beta}$. The infinite ground-state is thus unique.

We must start by proving that the only finite chain ground-states, are the ones we have built. The proof is done by induction on the size of the chain, using a procedure identical to what was done in the Majumdar-Ghosh case. We state the result in the form of a theorem:

Theorem 4 (The Ground-States of the finite chain AKLT Model):

Let φ^N be any ground-state of the N-spins AKLT Hamiltonian — $H^{(1,N)}_{AKLT}$. Then it can be written as:

$$\varphi^N = A^{\alpha\beta}\Omega^{(N)}_{\alpha\beta} \quad for\ N\ odd \tag{4.93}$$

$$\varphi^N = A^{\alpha}_{\beta}\Omega^{(N)\,\beta}_{\alpha} \quad for\ N\ even \tag{4.94}$$

Where $A^{\alpha\beta}$ are A^{α}_{β} are arbitrary complex numbers (apart from normalization constraints).

- **Proof of the Theorem 4**:

The Hamiltonian $H^{(1,N)}_{AKLT}$ can be written as a sum of non-negative two-body interactions (apart from an irrelevant shift):

$$H^{(1,N)}_{AKLT} = \sum_{i=1}^{N-1} H_i \tag{4.95}$$

Where $H_i = 2JP_2(i, i+1)$.

For the case $N = 2$, we have seen that the only ground-states are precisely $\Omega^{(2)}{}_{\alpha}^{\beta} = \psi_{\alpha\gamma}\psi^{\gamma\beta}$. The induction step will be based on the fact that any ground-state of $H_{AKLT}^{(1,N+1)}$, must be a common ground-state of $H_{AKLT}^{(1,N)}$ and H_N. We have then two cases:

- If N is odd:

On one hand, we require φ^{N+1} to be a ground-state of $H_{AKLT}^{(1,N)}$, i.e.:

$$\varphi^{N+1} = A_{\mu\nu}^{\alpha\beta}\Omega^{(N)}{}_{\alpha\beta}\psi^{\mu\nu} = A_{\mu\nu}^{\alpha\beta}\Omega^{(N-1)}{}_{\alpha}^{\gamma}\psi_{\gamma\beta}\psi^{\mu\nu} \tag{4.96}$$

On the other hand, we must also require it to be a also ground state of H_N, which means that:

$$\varphi^{N+1} = C_{\nu}^{\alpha}\Omega^{(N)}{}_{\alpha\beta}\psi^{\beta\nu} = C_{\nu}^{\alpha}\Omega^{(N-1)}{}_{\alpha}^{\gamma}\psi_{\gamma\beta}\psi^{\beta\nu} \tag{4.97}$$

Comparing (4.95) with (4.96), we need to have $A_{1\nu}^{\alpha 2} = A_{2\nu}^{\alpha 1} = 0$ and $A_{1\nu}^{\alpha 1} = A_{2\nu}^{\alpha 2} = C_{\nu}^{\alpha}$, which proves the result.

- If N is even:

In this case, requiring φ^{N+1} to be a ground-state of $H_{AKLT}^{(1,N)}$, gives[20]:

$$\varphi^{N+1} = A_{\beta}^{\alpha\,\mu\nu}\Omega^{(N)}{}_{\alpha}^{\beta}\psi_{\mu\nu} = A_{\beta}^{\alpha\,\mu\nu}\Omega^{(N-1)}_{\alpha\gamma}\psi^{\gamma\beta}\psi_{\mu\nu} \tag{4.98}$$

On the other hand, requiring it to be a ground state of H_N means that:

$$\varphi^{N+1} = C^{\alpha\nu}\Omega^{(N)}{}_{\alpha}^{\beta}\psi_{\beta\nu} = C^{\alpha\nu}\Omega^{(N-1)}_{\alpha\gamma}\psi^{\gamma\beta}\psi_{\beta\nu} \tag{4.99}$$

Again, we compare (4.97) with (4.98) and get that $A_{2}^{\alpha\,1\nu} = A_{1}^{\alpha\,2\nu} = 0$ and $A_{1}^{\alpha\,1\nu} = A_{2}^{\alpha\,2\nu} = C^{\alpha\nu}$. This proves the result.

□

Now, we can move on and prove that in the thermodynamic limit these different ground-states cannot be distinguished by local measurements. For that, let us prove the following theorem:

[20]Where we arbitrarily define $\Omega^{(1)}_{\alpha\gamma} \equiv \delta_{\alpha\gamma}$, just to allow the proof to work for all $N \geq 2$.

Theorem 5 (Ground-State Expectation Values in the Infinite Chain):

If we consider the (odd length) chain $\{-N, -N+1, ..., 0, ..., N-1, N\}$ with the AKLT Hamiltonian, and let A be an observable that acts non-trivially only in the sites $i \in \{-l, -l+1, ..., 0, ..., l-1, l\}$, for $l < N$.
Then, the following two expressions are true:

$$\lim_{N\to\infty} \left\{ \frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\alpha\beta}^{(2N+1)}\right)}{\left(\Omega_{\alpha\beta}^{(2N+1)}, \Omega_{\alpha\beta}^{(2N+1)}\right)} \right\} = \frac{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\gamma\delta}^{(2l+1)}\right)}{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, \Omega_{\gamma\delta}^{(2l+1)}\right)} \tag{4.100}$$

$$\lim_{N\to\infty} \left\{ \frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\mu\nu}^{(2N+1)}\right)}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\| \left\|\Omega_{\mu\nu}^{(2N+1)}\right\|} \right\} = 0 \quad if \quad \alpha \neq \mu \text{or } \beta \neq \nu, \tag{4.101}$$

Note: The way we have defined the sequence of systems converging to the thermodynamic limit, allow us never to worry about even length chains.

- **Proof of the Theorem 5:**
  - **Proof of (4.99):**

    We start by noting that, since the support of A is $\{-l, -l+1, ..., l-1, l\}$, we can write:

$$\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\alpha\beta}^{(2N+1)}\right) = \sum_{\gamma\delta\mu\nu} \left(\Omega^{(N-l)}{}_{\alpha}^{\gamma}, \Omega^{(N-l)}{}_{\alpha}^{\mu}\right) \left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\mu\nu}^{(2l+1)}\right) \left(\Omega^{(N-l)\delta}{}_{\beta}, \Omega^{(N-l)\nu}{}_{\beta}\right) \tag{4.102}$$

    And also,

$$\left(\Omega_{\alpha\beta}^{(2N+1)}, \Omega_{\alpha\beta}^{(2N+1)}\right) = \sum_{\gamma\delta\mu\nu} \left(\Omega^{(N-l)}{}_{\alpha}^{\gamma}, \Omega^{(N-l)}{}_{\alpha}^{\mu}\right) \left(\Omega_{\gamma\delta}^{(2l+1)}, \Omega_{\mu\nu}^{(2l+1)}\right) \left(\Omega^{(N-l)\delta}{}_{\beta}, \Omega^{(N-l)\nu}{}_{\beta}\right) \tag{4.103}$$

    From (4.85), we know that — $\left(\Omega^{(N-l)}{}_{\alpha}^{\gamma}, \Omega^{(N-l)}{}_{\alpha}^{\mu}\right) = \delta_{\alpha}^{\gamma}\delta_{\alpha}^{\mu} + \frac{1}{2}\left[3^{N-l}-1\right]\delta^{\gamma\mu}$ — with a similar expression for the last factor in (4.102). Hence, we can write the following:

$$\begin{aligned} &\frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\alpha\beta}^{(2N+1)}\right)}{\left(\Omega_{\alpha\beta}^{(2N+1)}, \Omega_{\alpha\beta}^{(2N+1)}\right)} = \\ &= \frac{\sum_{\gamma\delta\mu\nu}\left[\delta_{\alpha}^{\gamma}\delta_{\alpha}^{\mu} + \frac{1}{2}\left[3^{N-l}-1\right]\delta^{\gamma\mu}\right]\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\mu\nu}^{(2l+1)}\right)\left[\delta^{\delta}{}_{\beta}\delta^{\nu}{}_{\beta} + \frac{1}{2}\left[3^{N-l}-1\right]\delta^{\delta\nu}\right]}{\sum_{\gamma\delta\mu\nu}\left[\delta_{\alpha}^{\gamma}\delta_{\alpha}^{\mu} + \frac{1}{2}\left[3^{N-l}-1\right]\delta^{\gamma\mu}\right]\left(\Omega_{\gamma\delta}^{(2l+1)}, \Omega_{\mu\nu}^{(2l+1)}\right)\left[\delta^{\delta}{}_{\beta}\delta^{\nu}{}_{\beta} + \frac{1}{2}\left[3^{N-l}-1\right]\delta^{\delta\nu}\right]} \end{aligned} \tag{4.104}$$

In the thermodynamic limit ($N \to \infty$), the only terms that survive from (4.101) are the ones of the order unity in N, i.e.:

$$\lim_{N\to\infty}\left\{\frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\alpha\beta}^{(2N+1)}\right)}{\left(\Omega_{\alpha\beta}^{(2N+1)}, \Omega_{\alpha\beta}^{(2N+1)}\right)}\right\} = \lim_{N\to\infty}\left\{\frac{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\gamma\delta}^{(2l+1)}\right)}{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, \Omega_{\gamma\delta}^{(2l+1)}\right)}\right\} \tag{4.105}$$

– **Proof of (4.100):**

On the other hand, if calculate $\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\mu\nu}^{(2N+1)}\right)$, for $\alpha \neq \mu$ or $\beta \neq \nu$, we get the same kind of decomposition:

$$\begin{aligned}\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\mu\nu}^{(2N+1)}\right) &= \sum_{\gamma\delta\rho\sigma}\left(\Omega^{(N-l)}{}_{\alpha}^{\gamma}, \Omega^{(N-l)}{}_{\mu}^{\rho}\right)\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\rho\sigma}^{(2l+1)}\right)\left(\Omega^{(N-l)\delta}{}_{\beta}, \Omega^{(N-l)\sigma}{}_{\nu}\right) = \\ &= \sum_{\gamma\delta\rho\sigma}\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\rho\sigma}^{(2l+1)}\right)\delta_{\alpha}^{\gamma}\delta_{\mu}^{\rho}\delta_{\beta}^{\delta}\delta_{\nu}^{\sigma} = \left(\Omega_{\alpha\beta}^{(2l+1)}, A\Omega_{\mu\nu}^{(2l+1)}\right)\end{aligned} \tag{4.106}$$

But, in this case, the result does not depend on N, meaning that:

$$\lim_{N\to\infty}\left\{\frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\mu\nu}^{(2N+1)}\right)}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\|\left\|\Omega_{\mu\nu}^{(2N+1)}\right\|}\right\} = 0 \tag{4.107}$$

□

- **Proof of the Uniqueness of the AKLT state in the Infinite chain:**

The two theorems above finally allow us to see that all of the AKLT ground-states, will have the same expectation values for any local observable, in the limit $N \to \infty$. To prove it, we just need to write an arbitrary normalized ground-state for the chain $\{-N, ...N\}$:

$$\varphi^{(2N+1)} = C^{\alpha\beta}\frac{\Omega_{\alpha\beta}^{(2N+1)}}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\|} \tag{4.108}$$

The normalization condition for (4.107) can be written as:

$$1 = \left(\varphi^{(2N+1)}, \varphi^{(2N+1)}\right) = \sum_{\alpha\beta}\left|C^{\alpha\beta}\right|^2 + \sum_{(\alpha,\beta)\neq(\gamma,\delta)} C^{\alpha\beta}\left(C^{\gamma\delta}\right)^*\frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, \Omega_{\gamma\delta}^{(2N+1)}\right)}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\|\left\|\Omega_{\gamma\delta}^{(2N+1)}\right\|} \tag{4.109}$$

In the limit $N \to \infty$, the constraint (4.108) reduces to:

$$\sum_{\alpha\beta}\left|C^{\alpha\beta}\right|^2 = 1$$

Now, if we assume than an arbitrary local observable A (acting only on sites $\{-l, ..., l\}$]) is measured on the state $\varphi^{(2N+1)}$, its expectation value will be given by:

$$\langle A\rangle_{\varphi}^{(N)} = \left(\varphi^{(2N+1)}, A\varphi^{(2N+1)}\right) = \sum_{\alpha\beta} \left|C^{\alpha\beta}\right|^2 \frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\alpha\beta}^{(2N+1)}\right)}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\|^2} + \\ + \sum_{(\alpha,\beta)\neq(\gamma,\delta)} C^{\alpha\beta}\left(C^{\gamma\delta}\right)^* \frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\gamma\delta}^{(2N+1)}\right)}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\| \left\|\Omega_{\gamma\delta}^{(2N+1)}\right\|} \tag{4.110}$$

And according to the results of **Theorem 5**, each of the terms in the second summation go to zero in the thermodynamic limit. Using also (4.99) and the normalization condition, we get:

$$\langle A\rangle_{\varphi}^{(\infty)} = \sum_{\alpha\beta} \left|C^{\alpha\beta}\right|^2 \lim_{N\to\infty} \left\{ \frac{\left(\Omega_{\alpha\beta}^{(2N+1)}, A\Omega_{\alpha\beta}^{(2N+1)}\right)}{\left\|\Omega_{\alpha\beta}^{(2N+1)}\right\|^2} \right\} = \frac{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\gamma\delta}^{(2l+1)}\right)}{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, \Omega_{\gamma\delta}^{(2l+1)}\right)} \sum_{\alpha\beta} \left|C^{\alpha\beta}\right|^2 = \\ = \frac{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, A\Omega_{\gamma\delta}^{(2l+1)}\right)}{\sum_{\gamma\delta}\left(\Omega_{\gamma\delta}^{(2l+1)}, \Omega_{\gamma\delta}^{(2l+1)}\right)} \tag{4.111}$$

In conclusion, since (4.110) is independent of the coefficients $C^{\alpha\beta}$ (that define a particular ground-state φ), all the ground-states are undistinguishable by local measurements.

4.2.5. The Low-Energy Spectrum of the AKLT Model

Similarly to the case of the Majumdar-Ghosh Model, we can prove that there is an energy gap between the ground-state and the first excited states, that survives in the thermodynamic limit. For that, we write the AKLT Hamiltonian as a sum of non-negative 2-body operators. I.e.:

$$H_{AKLT}^{(m,n)} = \sum_{i=m}^{n-1} H_i \tag{4.112}$$

Again, we can formalize this by the following theorem:

Theorem 6 (The AKLT Model is Gapped):

For any state $\psi \in \mathscr{H}$ orthogonal to the ground-state manifold of the AKLT model — $H^{(N)}_{AKLT}$ — we have the following inequality:

$$\left(\psi, H^{(1,N)}_{AKLT}\psi\right) \geq \Delta_{AKLT}\left(\psi,\psi\right) \tag{4.113}$$

Where $\Delta_{AKLT} > 0$ is a positive number independent of N.

To prove this theorem, we will proceed in a manner similar to what was done for the Majumdar-Ghosh model. Starting by same definitions:

1. Q_n will be the projector onto the ground-states of $H^{(1,n)}_{AKLT}$;
2. $P_n = \mathbb{I} - Q_n$ is its complementary;
3. $Q_{i,j}$ will be the projector onto the states of $H^{(i,j)}_{AKLT}$;

From the construction of the AKLT states, it is also easy to see that [Figure 4.7]:

$$\dim\left[Im\left\{Q_k - Q_{k+1}\right\}\right] = 8 \tag{4.114}$$

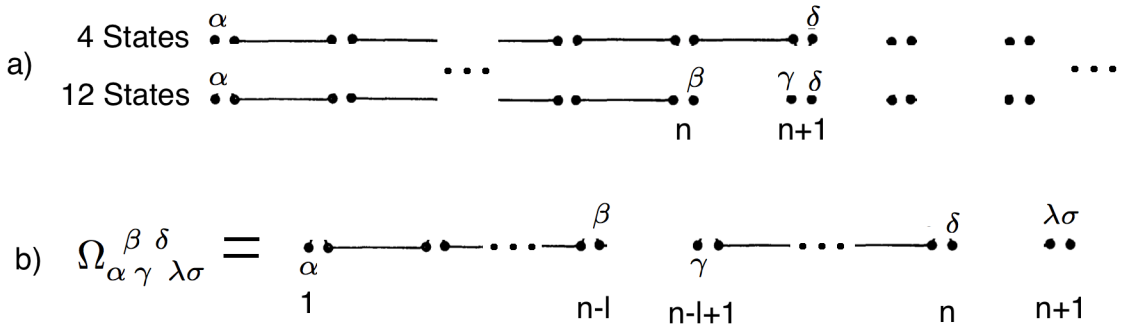


Figure 4.7.: a) Graphical representation of the ground-states of $H^{(1,n+1)}_{AKLT}$ (on the top) and $H^{(1,n)}_{AKLT}$ (on the bottom). Here it is evident that in the former case, the state on the site $n+1$ can be any, since it will not contribute to the energy. Therefore, in this case, besides the 4 possible choices for the edge spins in the $\{1,n\}$ chain, there is a 3-fold degeneracy (3 states of the spin-1 representation) due to the site $n+1$. b) Definition of the state $\Omega^{\beta\ \delta}_{\alpha\ \gamma\ \lambda\sigma}$ used in the proof of Lemma 9.

Like before, we use the set — $\{\varphi^i_k\}_i$, $i \in \{1,...,8\}$ — as an orthonormal basis for the space $Im\left[Q_k - Q_{k+1}\right]$ and define the following:

$$\psi^i_{n+1} \in \mathscr{H} \equiv \frac{Q_{n-l+1,n+1}\varphi^i_{n+1}}{\left\|Q_{n-l+1,n+1}\varphi^i_{n+1}\right\|}. \tag{4.115}$$

$$\varepsilon(l) \equiv \sup_n \max_i \left\| Q_{n-l+1,n+1} \varphi^i_{n+1} \right\|^2 . \tag{4.116}$$

Where $l < n$ is an integer to be chosen in the end.

- **The Fundamental Inequality for the AKLT Model:**

We can notice that the fundamental inequality (4.54) is also true in this case. In fact, the proof we have given in the last section, did not assume any specific property of the Majumdar-Ghosh model, other than the fact that $H^{(1,n)}$ is a sum of local positive terms and that any ground-state of $H^{(1,n)}$ is also a ground-state of $H^{(1,m)}$ (if $m \leq n$). All of these statements remain true for the AKLT model, so one may just recover the referred inequality, as follows:

$$\begin{aligned} \sum_{n=l}^{N-1} (P_{n+1} - P_n) &\leq 3(l+1) \max \left\{ dim \left[Q_k - Q_{k+1} \right] \right\} \varepsilon(l) + \frac{3(l+1)}{\epsilon_{l-1}} H^{(1,N)}_{AKLT} = \\ &= 24(l+1)\varepsilon(l) + \frac{3(l+1)}{\epsilon_{l-1}} H^{(1,N)}_{AKLT} \end{aligned} \tag{4.117}$$

Where ϵ_{l+1} is the first non-zero eigenvalue of $H^{(1,l+1)}_{AKLT}$, and use was made of the fact (4.113).

Also, we know that $P_N = \sum_{k=l}^{N-1} (P_{k+1} - P_k) + P_l$ and $P_l \leq \frac{1}{\epsilon_l} H^{(1,l)}_{AKLT} \leq \frac{1}{\epsilon_l} H^{(1,L)}_{AKLT}$, and that allow us to establish the following Lemma:

Lemma 5 (Fundamental Inequality for the AKLT Model):

For the AKLT model in the chain with N spins, the following inequality is true for any state ψ orthogonal to the ground-state manifold:

$$\left[1 - 24(l+1)\varepsilon_{AKLT}(l) \right] (\psi, \psi) \leq \left(\frac{3(l+1)}{\epsilon_{l-1}} + \frac{1}{\epsilon_l} \right) \left(\psi, H^{(1,N)}_{AKLT} \psi \right) \tag{4.118}$$

Where l is an arbitrary integer in $\{1, ..., N-1\}$, $\epsilon_l / \epsilon_{l+1}$ are the lowest non-zero eigenvalues of $H^{(1,l)}_{AKLT} / H^{(1,l+1)}_{AKLT}$ and $\varepsilon_{AKLT}(l) \equiv \sup_n \max_i \left\| Q_{n-l+1,n+1} \varphi^i_{n+1} \right\|^2$.

Finally, we can use the inequality (4.117) to prove that the model is gapped, provided that it is possible to find an integer l, such that:

$$24(l+1)\varepsilon_{AKLT}(l) < 1$$

.

In fact, we can prove the following bound:

Lemma 6 (The ε_{AKLT} bound) :

For the AKLT model, and defining $\varepsilon_{AKLT}(l) = \sup_n \max_i \left\| Q_{n-l+1,n+1}\varphi^i_{n+1} \right\|^2$, we can see that, for every integer l:

$$\varepsilon_{AKLT}(l) \lesssim 3^{-l} \tag{4.119}$$

- **Proof of Lemma 6**[21]:

To prove this statement, we must start by writing φ as being one of the elements of the set $\{\varphi^i_{n+1}\}_i$. Using the basis defined in Figure 4.7 b), it can be written as follows:

$$\varphi = A^{\alpha\ \delta\sigma}_{\gamma} \Omega_{\alpha\ \beta\ \delta\sigma}^{\ \beta\ \gamma} \tag{4.120}$$

Where $A^{\alpha\ \rho\sigma}_{\delta}$ are complex coefficients which are symmetrical in the exchange of the last 2 indices. The normalization condition, given as [Appendix D.3]:

$$(\varphi,\varphi) = 2\sum_{\delta\sigma}\left|\sum_{\alpha} A^{\alpha\ \delta\sigma}_{\alpha}\right|^2 + (3^n-1)\sum_{\alpha\gamma\delta\sigma}\left|A^{\alpha\ \delta\sigma}_{\gamma}\right|^2 = 1 \tag{4.121}$$

And since (4.120) is a sum of positive numbers, it implies the following orders of magnitude its the last terms:

$$\left|A^{\alpha\ \delta\sigma}_{\gamma}\right| \sim 3^{-\frac{n}{2}} \tag{4.122}$$

On the other hand, φ is orthogonal to any ground-state of $H^{(1,n+1)}_{AKLT}$, meaning that the following expression holds [Appendix D.3]:

$$\left(\Omega_{\alpha\ \beta\ \gamma\delta}^{\ \beta\ \gamma}, \varphi\right) = 0 \Leftrightarrow 2A^{\mu}_{\mu\ \alpha\delta} + (3^n-1)A^{\gamma}_{\alpha\ \gamma\delta} = 0 \tag{4.123}$$

Yielding:

$$\left|A^{\gamma}_{\alpha\ \gamma\delta}\right| = \frac{2}{3^n-1}\left|A^{\mu}_{\mu\ \alpha\delta}\right| \tag{4.124}$$

We also know that $Q_{n-l+1,n+1}\varphi$ is a ground-state of both $H^{(n-l+1,n+1)}_{AKLT}$ (by definition) and $H^{(1,n-l)}_{AKLT}$[22]. Consequently, we can write this state as:

[21] The proof supposes n and $l$to be even integers, but it can be easily generalized to all the other cases.

[22] Since the commutator $\left[H^{(1,n-l)}_{AKLT}, Q_{n-l+1,n+1}\right] = 0$ and φ is a ground-state of $H^{(1,n-l)}_{AKLT}$

$$Q_{n-l+1,n+1}\varphi = C_{\beta}^{\alpha\,\gamma\sigma}\frac{\Omega_{\alpha\,\gamma\;\delta\sigma}^{\beta\;\delta}}{\left\|\Omega_{\alpha\,\gamma\;\delta\sigma}^{\beta\;\delta}\right\|} = D_{\beta}^{\alpha\,\gamma\sigma}\Omega_{\alpha\,\gamma\;\delta\sigma}^{\beta\;\delta} \tag{4.125}$$

Where the coefficients $C_{\beta}^{\alpha\,\gamma\sigma}$ obey $\left|C_{\beta}^{\alpha\,\gamma\sigma}\right| \lesssim 1 \Rightarrow \left|D_{\beta}^{\alpha\,\gamma\sigma}\right| \lesssim 3^{-n/2}$[23].

In the end, what we need calculate is $\|Q_{n-l+1,n+1}\varphi\|^2 = (\varphi, Q_{n-l+1,n+1}\varphi)$, so we can use expressions (4.119) and (4.124) to write this overlap [Appendix D.3]:

$$\begin{aligned}(\varphi, Q_{n-l+1,n+1}\varphi) &= \left|D_{\beta}^{\alpha\,\gamma\sigma}A_{\nu}^{\mu\,\rho\epsilon}\left(\Omega_{\mu\,\lambda}^{\lambda\;\nu}{}_{\rho\epsilon}, \Omega_{\alpha\,\gamma\;\delta\sigma}^{\beta\;\delta}\right)\right| = \left|2D_{\delta}^{\delta\,\beta\gamma}A_{\alpha\,\beta\gamma}^{\alpha} + (3^l-1)D_{\beta}^{\alpha\,\gamma\delta}A_{\alpha\,\gamma\delta}^{\beta} + \right. \\ &= +(3^{n-l}-1)D_{\delta}^{\delta\,\alpha\gamma}A_{\alpha\,\beta\gamma}^{\beta} + \frac{1}{2}(3^{n-l}-1)(3^l-1)D_{\delta}^{\alpha\,\delta\gamma}A_{\alpha\,\beta\gamma}^{\beta}\Big| \leq \left|D_{\delta}^{\delta\,\beta\gamma}\right|\left|A_{\alpha\,\beta\gamma}^{\alpha}\right| + \\ &+ (3^l-1)\left|D_{\beta}^{\alpha\,\gamma\delta}\right|\left|A_{\alpha\,\gamma\delta}^{\beta}\right| + (3^{n-l}-1)\left|D_{\delta}^{\delta\,\alpha\gamma}\right|\left|A_{\alpha\,\beta\gamma}^{\beta}\right| + \frac{1}{2}(3^{n-l}-1)(3^l-1)\left|D_{\delta}^{\alpha\,\delta\gamma}\right|\left|A_{\alpha\,\beta\gamma}^{\beta}\right|\end{aligned} \tag{4.126}$$

From (4.125) one sees that $\left|D_{\beta}^{\alpha\,\gamma\delta}\right|\left|A_{\alpha\,\gamma\delta}^{\beta}\right| \sim 3^{-n}$. On the other hand, the rest of the terms can be re-written using equation (4.123), as follows:

$$\begin{aligned}&\left|D_{\delta}^{\delta\,\beta\gamma}\right|\left|A_{\alpha\,\beta\gamma}^{\alpha}\right| + (3^{n-l}-1)\left|D_{\delta}^{\delta\,\alpha\gamma}\right|\left|A_{\alpha\,\beta\gamma}^{\beta}\right| + \frac{1}{2}(3^{n-l}-1)(3^l-1)\left|D_{\delta}^{\alpha\,\delta\gamma}\right|\left|A_{\alpha\,\beta\gamma}^{\beta}\right| = \\ &= \left|D_{\delta}^{\delta\,\alpha\gamma}\right|\left|A_{\mu\,\alpha\gamma}^{\mu}\right| + (3^{n-l}-1)\left|D_{\delta}^{\delta\,\alpha\gamma}\right|\frac{2}{3^n-1}\left|A_{\mu\,\alpha\gamma}^{\mu}\right| + \frac{1}{2}(3^{n-l}-1)(3^l-1)\left|D_{\delta}^{\alpha\,\delta\gamma}\right|\frac{2}{3^n-1}\left|A_{\mu\,\alpha\gamma}^{\mu}\right| = \\ &= \left|A_{\mu\,\alpha\gamma}^{\mu}\right|\left|D_{\delta}^{\delta\,\alpha\gamma}\right| \times \left\{1 + \frac{2(3^{n-l}-1)}{3^n-1}\right\} + \left|A_{\mu\,\alpha\gamma}^{\mu}\right|\left|D_{\delta}^{\alpha\,\delta\gamma}\right|\frac{(3^{n-l}-1)(3^l-1)}{3^n-1} \lesssim \\ &\lesssim \left|A_{\mu\,\alpha\gamma}^{\mu}\right|\left|D_{\delta}^{\delta\,\alpha\gamma}\right|\left\{1+3^{-l}\right\} + \left|A_{\mu\,\alpha\gamma}^{\mu}\right|\left|D_{\delta}^{\alpha\,\delta\gamma}\right| \lesssim 3^{-n}\end{aligned}$$

Finally, we can see that $\varepsilon_{AKLT}(l) = \|Q_{n-l+1,n+1}\varphi\|^2 \lesssim 3^{-n} \lesssim 3^{-l}$, as we wanted to prove.

□

- **Proof of the Theorem 6:**

It is clear that Lemma 6 ensure that there are integers $l < N$, such that $24(l+1)\varepsilon_{AKLT}(l) < 1$. Let l_C be one of those values of l, then the inequality (4.117) yields the final result:

$$\begin{aligned}\left[1 - 24(l_C+1)\varepsilon_{AKLT}(l_C)\right](\psi,\psi) &\leq \left(\frac{3(l_C+1)}{\epsilon_{l_C-1}} + \frac{1}{\epsilon_{l_C}}\right)\left(\psi, H_{AKLT}^{(1,N)}\psi\right) \Rightarrow \\ &\Rightarrow \left(\psi, H_{AKLT}^{(1,N)}\psi\right) \geq \Delta_{AKLT}(\psi,\psi)\end{aligned} \tag{4.127}$$

[23]Notice that $\left(\Omega_{\alpha\,\gamma\;\delta\sigma}^{\beta\;\delta}, \Omega_{\alpha\,\gamma\;\delta\sigma}^{\beta\;\delta}\right) = \left(\Omega^{(n-l)\;\beta}_{\alpha}, \Omega^{(n-l)\;\beta}_{\alpha}\right)\left(\Omega^{(l)}{}_{\gamma\sigma}, \Omega^{(l)}{}_{\gamma\sigma}\right) =\sim 3^{n-l+l} = 3^n$.

Where ψ is any state of $\mathscr{H}$ that is orthogonal to the ground-state, and

$$\Delta_{AKLT} = \frac{1 - 24(l_C + 1)\varepsilon_{AKLT}(l_C)}{\frac{3(l_C+1)}{\epsilon_{l_C-1}} + \frac{1}{\epsilon_{l_C}}} > 0$$

This proves that the system is, indeed, gapped.

4.2.6. The Schwinger Boson representation of the AKLT state

References: [7, 33, 34]

Up till now, we have proved a series of properties associated with the ground-state of the AKLT model, by using a very clever tensor notation that made the expression of the complex wavefunction, as compact as possible.

In this section, we will prove that it is possible to express the AKLT ground-states in terms of Schwinger bosonic operators, as was first noticed by D. P. Arovas, A. Auerbach and F. D. M. Haldane [33]. This new representation can also be used to remake the calculations already done. However, its main relevance is fact that it allows for easy generalizations of the VBS construction to higher-dimensional lattices and different localized spins.

The Schwinger representation was introduced in chapter 2, so we merely restate the important definitions:

$$S_i^+ = a_i^\dagger b_i \quad S_i^- = b_i^\dagger a_i \quad S_i^z = 1/2 \left\{ a_i^\dagger a_i - b_i^\dagger b_i \right\} \tag{4.128}$$

$$\left[a_i, a_j^\dagger\right] = \left[b_i, b_j^\dagger\right] = \delta_{ij} \quad [a_i, a_j] = [b_i, b_j] = [a_i, b_j] = \left[a_i, b_j^\dagger\right] = 0$$

Knowing also that the quantum numbers s and m for the local spin states are related to the occupation numbers of the a- and b-bosons, as follows — $s_i = 1/2 \left(n_a^i + n_b^i\right) \quad and \quad m_i = 1/2 \left(n_a^i - n_b^i\right)$. Using these facts, it is easy to write the standard spin basis states of a site $i \in \mathscr{L}$, as follows:

$$|s, m\rangle_i = \frac{\left(a_i^\dagger\right)^{s+m} \left(b_i^\dagger\right)^{s-m}}{\sqrt{(s+m)!\,(s-m)!}} |0, 0\rangle_i \tag{4.129}$$

From (4.128), it is clear that the local states — $\psi_{\alpha\beta}$ — can be written in terms of these bosonic operators as follows:

$$\psi_{11} = \psi^{22} = a^\dagger a^\dagger |0, 0\rangle \quad ; \quad \psi_{22} = \psi^{11} = b^\dagger b^\dagger |0, 0\rangle \quad ; \quad \psi_{12} = \psi_{21} = -\psi^{12} = a^\dagger b^\dagger |0, 0\rangle \tag{4.130}$$

Finally, to represent the AKLT states using this language, we must start by dealing with only one bond in the chain [Figure 4.5 c)]. The ground-state for the projector $P_2(i, i+1)$ is obtained by guaranteeing

that two of the virtual spins are in a singlet state along the bond, so one of the possibilities is[24]:

$$a_i^\dagger \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right) a_{i+1}^\dagger \left|\omega\right\rangle = \left(a_i^\dagger\right)^2 b_{i+1}^\dagger a_{i+1}^\dagger \left|\omega\right\rangle - a_i^\dagger b_i^\dagger \left(a_{i+1}^\dagger\right)^2 \left|\omega\right\rangle \tag{4.131}$$

Using the identifications in (4.129), we get:

$$a_i^\dagger \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right) a_{i+1}^\dagger \left|\omega\right\rangle = -\psi_{11}\psi^{12} - \psi_{12}\psi^{22} = -\psi_{1\alpha}\psi^{\alpha 2} \tag{4.132}$$

This last result can be trivially generalized to a finite chain with N sites. If we suppose, with no loss of generality, that N is an odd number, then the four AKLT ground-states can be written as follows:

$$\Omega_{11}^{(N)} = a_1^\dagger \left[\prod_{i=1}^{N} \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)\right] a_N^\dagger \left|\omega\right\rangle \tag{4.133}$$

$$\Omega_{22}^{(N)} = b_1^\dagger \left[\prod_{i=1}^{N} \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)\right] b_N^\dagger \left|\omega\right\rangle \tag{4.134}$$

$$\Omega_{12}^{(N)} = a_1^\dagger \left[\prod_{i=1}^{N} \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)\right] b_N^\dagger \left|\omega\right\rangle \tag{4.135}$$

$$\Omega_{21}^{(N)} = b_1^\dagger \left[\prod_{i=1}^{N} \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)\right] a_N^\dagger \left|\omega\right\rangle \tag{4.136}$$

If we are interested in the infinite chain, then the (unique) ground-state wavefunction is written in an even more symmetrical form:

$$\left|AKLT_\infty\right\rangle = \prod_{i=-\infty}^{\infty} \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right) \left|\omega\right\rangle \tag{4.137}$$

The expression (4.136) for the one-dimensional AKLT ground-state will be useful in many ways. For a start, it makes explicit its rotational invariance. By using the transformation law for the Schwinger Bosons [Appendix C.1], for a rotation parametrized by the Euler angles (θ, ϕ):

$$\begin{cases} \tilde{a}_i^\dagger = e^{-i\phi/2} \cos\left(\theta/2\right) a_i^\dagger + e^{i\phi/2} \sin\left(\theta/2\right) b_i^\dagger \\ \tilde{b}_i^\dagger = -e^{-i\phi/2} \sin\left(\theta/2\right) a_i^\dagger + e^{i\phi/2} \cos\left(\theta/2\right) b_i^\dagger \end{cases} \tag{4.138}$$

We can see that the combination $\left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)$ is an invariant under any rotation — $U(\theta, \phi)$ (Details in the [Appendix C.4]):

$$U(\theta,\phi) \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right) U^\dagger(\theta,\phi) = \tilde{a}_i^\dagger \tilde{b}_{i+1}^\dagger - \tilde{a}_{i+1}^\dagger \tilde{b}_i^\dagger = a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger \tag{4.139}$$

[24] In every expression that follows, the state $\left|\omega\right\rangle$ stands for the common vacuum of a- and b-bosons in every site of the lattice. I.e. $\left|\omega\right\rangle = \otimes_{i\in\mathscr{L}} \left|0,0\right\rangle_i$.

Finally, we can write[25]:

$$U^{\dagger}(\theta,\phi)\,|AKLT_{\infty}\rangle = \prod_{i=-\infty}^{\infty} U^{\dagger}(\theta,\phi)\left(a_i^{\dagger}b_{i+1}^{\dagger} - a_{i+1}^{\dagger}b_i^{\dagger}\right)U^{\dagger}(\theta,\phi)U(\theta,\phi)\,|\omega\rangle = |AKLT_{\infty}\rangle \tag{4.140}$$

So, the state $|AKLT_{\infty}\rangle$ is invariant under any rotation, as expected from the previous discussions.

4.2.7. Calculations of Correlation functions using a Spin Coherent-State Representation

Using the representation (4.136) for the VBS state, we will recalculate the spin-spin correlation functions. For doing that, we must find a way to represent the 1-D AKLT state in terms of the coherent state basis — $\left|\hat{\Omega}\right\rangle$ — defined in chapter 3. The main properties of this basis are restated as follows:

- They are defined as follows (with $u_i(\theta_i,\phi_i) = e^{-i\phi_i/2}\cos\theta_i/2$ and $v_i(\theta_i,\phi_i) = e^{i\phi_i/2}\sin\theta_i/2$):

$$|\Omega^s\rangle = \prod_{i\in\mathscr{L}} \frac{\left(u_i a_i^{\dagger} + v_i b_i^{\dagger}\right)^{2s}}{\sqrt{(2s)!}}\,|\omega\rangle \tag{4.141}$$

- They obey a closure relation, altered with an appropriate measure of integration (for a lattice with N spins-s):

$$\mathbb{I} = \left(\frac{2s+1}{4\pi}\right)^N \int d\Omega\,|\Omega^s\rangle\,\langle\Omega^s| \tag{4.142}$$

- They form a non-orthogonal overcomplete basis, with a metric given by[26]:

$$\begin{aligned}\langle\Omega_2 \mid \Omega_1\rangle = \prod_{i\in\mathcal{L}}\left\langle\hat{\Omega}_{2i}^s \mid \hat{\Omega}_{1i}^s\right\rangle = \prod_{i\in\mathcal{L}}\left[\frac{1+\hat{\Omega}_{1i}\cdot\hat{\Omega}_{2i}}{2}\right]^S \times \\ \times \exp\left[2si\arctan\left\{\tan\left(\frac{\phi_{2i}-\phi_{1i}}{2}\right)\frac{\cos\left(\frac{\theta_{1i}+\theta_{2i}}{2}\right)}{\cos\left(\frac{\theta_{1i}-\theta_{2i}}{2}\right)}\right\}\right]\end{aligned} \tag{4.143}$$

- The spin operators have a very simple representation in this basis:

$$\vec{\mathbf{S}}_i = \left(\frac{2s+1}{4\pi}\right)^N (s+1)\int d\Omega\vec{\mathbf{\Omega}}_i\,|\Omega^s\rangle\,\langle\Omega^s| \tag{4.144}$$

Using the above properties, we can calculate the wavefunction associated with the AKLT ground-state, in the space of coherent-state parameters. For simplicity of discussion, we assume to be working in an even length chain with periodic boundary conditions. Hence, we have:

$$|AKLT_N\rangle = \left(a_N^{\dagger}b_1^{\dagger} - a_1^{\dagger}b_N^{\dagger}\right)\prod_{k=1}^{N}\left(a_i^{\dagger}b_{i+1}^{\dagger} - a_{i+1}^{\dagger}b_i^{\dagger}\right)|\omega\rangle \tag{4.145}$$

[25] By definition, the vacuum of the Schwinger Bosons is a singlet state.
[26] Where (ϕ_i,θ_i) are the Euler angles that define the direction of the unit vector $\hat{\Omega}_i$

The corresponding continuous wavefunction is:

$$\Psi^N_{AKLT}(\Omega) = \langle AKLT_N \mid \Omega\rangle^* = \langle\omega| \left(a_N b_1 - a_1 b_N\right) \prod_{k=1}^{N} \left(a_i b_{i+1} - a_{i+1} b_i\right) \prod_{i=1}^{N} \frac{\left(u_i a_i^\dagger + v_i b_i^\dagger\right)^{2s}}{\sqrt{(2s)!}} |\omega\rangle^* \Rightarrow$$

$$\Psi^N_{AKLT}(\Omega) = 2^N \left(u_N^* v_1^* - u_1^* v_N^*\right) \prod_{k=1}^{N} \left(u_i^* v_{i+1}^* - u_{i+1}^* v_i^*\right) \tag{4.146}$$

The first thing we must do with (4.145) is calculating the norm of the state $|AKLT_N\rangle$. That can be done using the resolution of identity (4.141), as follows:

$$\begin{aligned}\langle AKLT_N \mid AKLT_N\rangle &= \left(\frac{2s+1}{4\pi}\right)^N \int d\Omega \, \langle AKLT_N \mid \Omega\rangle \, \langle \Omega \mid AKLT_N\rangle = \\ &= \left(\frac{2s+1}{4\pi}\right)^N \int d\Omega \left|\Psi^N_{AKLT}(\hat{\Omega})\right|^2 \end{aligned} \tag{4.147}$$

The absolute value of Ψ^N_{AKLT} is easily seen to be[27]:

$$\left|\Psi^N_{AKLT}(\Omega)\right| = 2^N \sqrt{\frac{1-\hat{\Omega}_1\cdot\hat{\Omega}_N}{2}} \prod_{i=1}^{N} \sqrt{\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}}{2}} \tag{4.148}$$

Which means that:

$$\langle AKLT_N \mid AKLT_N\rangle = \left[\prod_{i=1}^{N} \int_{S^2} \frac{(2s+1)}{4\pi} d\Omega_i\right] \left(\frac{1-\hat{\Omega}_1\cdot\hat{\Omega}_N}{2}\right) \prod_{i=1}^{N} \left(\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}}{2}\right) \tag{4.149}$$

Now, the calculation of (4.148) may seem like an herculean task, but following the suggestion given in [33], we can take advantage of the fact that the lattice is one-dimensional, and integrate (4.148) iteratively along the periodic chain.

For that. we just have to notice the following basic result[28]:

$$\int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_2 \frac{\left(1-\hat{\Omega}_1\cdot\hat{\Omega}_2\right)\left(a \pm \hat{\Omega}_2\cdot\hat{\Omega}_3\right)}{4} = \frac{2s+1}{6} \frac{\left(3a \mp \hat{\Omega}_1\cdot\hat{\Omega}_3\right)}{2} \tag{4.150}$$

Now, using (4.149), we can do all the integrations in (4.148), starting from $\hat{\Omega}_2$, as follows:

[27] Note that $\hat{\Omega}_i\cdot\hat{\Omega}_j = \cos\theta_i/2\cos\theta_j/2 + \cos\left(\phi_i-\phi_j\right)\sin\theta_i/2\sin\theta_j/2$. Furthermore, there is also a factor of 2! for each term in the product due to the normalization of the Schwinger bosons Fock states as seen in Chapter 3.

[28] This result was obtained using Mathematica symbolic integration capabilities.

$$
\begin{aligned}
&\langle AKLT_N \mid AKLT_N\rangle = \\
&= 2^N \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_1 \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_2 \left(\frac{1-\hat{\Omega}_1\cdot\hat{\Omega}_2}{2}\right)\left(\frac{1-\hat{\Omega}_2\cdot\hat{\Omega}_3}{2}\right)(...) = \\
&= 2^N \left(\frac{2s+1}{6}\right) \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_1 \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_3 \left(\frac{3+\hat{\Omega}_1\cdot\hat{\Omega}_3}{2}\right)\left(\frac{1-\hat{\Omega}_3\cdot\hat{\Omega}_4}{2}\right)(...) = \\
&... = 2^N \left(\frac{2s+1}{6}\right)^{N-2} \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_1 \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_N \left(\frac{1-\hat{\Omega}_1\cdot\hat{\Omega}_N}{2}\right)\left(\frac{3^{N-2}-\hat{\Omega}_1\cdot\hat{\Omega}_N}{2}\right) = \\
&= 2^N \left(\frac{2s+1}{6}\right)^{N-1} \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_1 \left(\frac{3^{N-1}+\hat{\Omega}_1\cdot\hat{\Omega}_1}{2}\right) = \left(\frac{(2s+1)}{3}\right)^N \left[3^N+3\right]
\end{aligned}
$$

If one takes $s=1$, we get back the result already known — $\langle AKLT_N \mid AKLT_N\rangle = \left[3^N+3\right]$.

To calculate the spin-spin correlation function, we must also obtain the matrix element $\langle AKLT_N|\, \overrightarrow{\mathbf{S}}_0 \cdot \overrightarrow{\mathbf{S}}_r \,|AKLT_N\rangle$. Fortunately, this can be done by noticing that the operator $\overrightarrow{\mathbf{S}}_1 \cdot \overrightarrow{\mathbf{S}}_r$ has a very simple expression in terms of the coherent state basis, i.e.[29]:

$$
\overrightarrow{\mathbf{S}}_1 \cdot \overrightarrow{\mathbf{S}}_r = \left(\frac{2s+1}{4\pi}\right)^N (s+1)^2 \int d\Omega \overrightarrow{\mathbf{\Omega}}_1 \cdot \overrightarrow{\mathbf{\Omega}}_r \,|\Omega\rangle\langle\Omega| \tag{4.151}
$$

Then, the expression we want to calculate is:

$$
\begin{aligned}
\langle AKLT_N|\, \overrightarrow{\mathbf{S}}_0 \cdot \overrightarrow{\mathbf{S}}_r \,|AKLT_N\rangle = (s+1)^2 &\left[\prod_{i=1}^{N} \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_i\right] \overrightarrow{\mathbf{\Omega}}_1 \cdot \overrightarrow{\mathbf{\Omega}}_r \times \\
&\times \left(\frac{1-\hat{\Omega}_1\cdot\hat{\Omega}_N}{2}\right) \prod_{i=1}^{N} \left(\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}}{2}\right)
\end{aligned} \tag{4.152}
$$

Looking at (4.151), we notice that the only difference from (4.149) are the integrals over $\hat{\Omega}_1$ and $\hat{\Omega}_r$. So all the others can be done in exactly the same manner, by using (4.149). After doing that, we remain with the following:

$$
\begin{aligned}
(2s!)^N \left(\frac{2s+1}{6}\right)^{N-2} &\int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_1 \int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_r \overrightarrow{\mathbf{\Omega}}_1 \cdot \overrightarrow{\mathbf{\Omega}}_r \times \\
&\times \left(\frac{3^{r-2}-(-1)^r\hat{\Omega}_1\cdot\hat{\Omega}_r}{2}\right)\left(\frac{3^{N-r}+(-1)^r\hat{\Omega}_1\cdot\hat{\Omega}_r}{2}\right)
\end{aligned}
$$

Now, to perform the integral over $\hat{\Omega}_r$, we must resort to another basic analytical result:

[29] This is a simple generalization of the result stated in (4.143) and was already used in Chapter 3, to obtain the path-integral description of the Heisenberg model.

$$\int_{S^2} \frac{(2s+1)}{4\pi} d\hat{\Omega}_2 \hat{\Omega}_1 \cdot \hat{\Omega}_2 \frac{\left(a \pm \hat{\Omega}_1 \cdot \hat{\Omega}_2\right)\left(b \mp \hat{\Omega}_1 \cdot \hat{\Omega}_2\right)}{4} = \mp \frac{2s+1}{12}(a-b) \tag{4.153}$$

If we apply (4.152) to the above integral, we get:

$$(-1)^r (2s!)^N \left(\frac{2s+1}{6}\right)^N \left(3^{r-1} - 3^{N-r+1}\right) \tag{4.154}$$

Finally, the correlation function is found to be:

$$\begin{aligned} C^s_{AKLT}(r-1) &= \frac{\langle AKLT_N | \overrightarrow{\mathbf{S}}_0 \cdot \overrightarrow{\mathbf{S}}_r | AKLT_N \rangle}{\langle AKLT_N \mid AKLT_N \rangle} = \\ &= (s+1)^2 \frac{(-1)^r \left(3^{r-1} - 3^{N-r+1}\right)}{3^N + 3} \underset{N\to\infty}{\longmapsto} (-1)^{r-1}(s+1)^2 3^{-(r-1)} \end{aligned} \tag{4.155}$$

And the final result, for any integer s[30] in the one-dimensional chain is $C^s_{AKLT}(r) = (-1)^r (s+1)^2 3^{-r}$. This is the same as (4.91) when one takes $s = 1$, and sums over all the indices.

Before embarking on a new subject, we take the advantage of this discussion to point out that the above calculation is not exclusive of the correlation functions. In fact, we have proven a Theorem by Kutzner (in Chapter 3), which indicated us that any local observable A, can be given a diagonal representation in the coherent-state basis:

$$A = \left(\frac{2s+1}{4\pi}\right)^N \int d\Omega \mathscr{A}(\Omega) |\Omega\rangle \langle\Omega| \tag{4.156}$$

And this means that the average of the observable in the state $|AKLT_N\rangle$ has the form:

$$\langle A \rangle_{AKLT} = \frac{\langle AKLT_N | A | AKLT_N \rangle}{\langle AKLT_N \mid AKLT_N \rangle} = \left(\frac{2s+1}{4\pi}\right)^N \int d\Omega \mathscr{A}(\Omega) \left|\Psi^N_{AKLT}(\Omega)\right|^2 \tag{4.157}$$

The first thing we can say about (4.156) is that similar techniques to the ones used above, can be also applied for any local average. But more importantly, we notice that:

$$\begin{aligned} \left|\Psi^N_{AKLT}(\Omega)\right|^2 &= \frac{1 - \hat{\Omega}_1 \cdot \hat{\Omega}_N}{2} \prod_{i=1}^{N} \frac{1 - \hat{\Omega}_i \cdot \hat{\Omega}_{i+1}}{2} = \\ &= (constant) \times \exp\left[\sum_{i=1}^{N} \left(\ln\left\{1 - \hat{\Omega}_i \cdot \hat{\Omega}_{i+1}\right\}\right) + \ln\left\{1 - \hat{\Omega}_1 \cdot \hat{\Omega}_N\right\}\right] \end{aligned} \tag{4.158}$$

So this means that the calculation of any physical quantity in the AKLT state (at $T = 0$), is equivalent of calculating an average in a classical system with the following local Hamiltonian:

[30] Obviously that, if $s > 1$, the corresponding VBS state (144) will not be a ground-state of H_{AKLT}, but instead of an appropriate Hamiltonian - $H = \sum_i P_{2s}(i, i+1)$.

$$H_{cl} = \sum_{i=1}^{N} \ln\left\{1 - \hat{\Omega}_i \cdot \hat{\Omega}_{i+1}\right\}^{-1} + \ln\left\{1 - \hat{\Omega}_1 \cdot \hat{\Omega}_N\right\}^{-1} \tag{4.159}$$

This is another example of a mapping between a zero-temperature quantum model, and a finite temperature classical model[31]. This fact was first pointed out in Ref. [33] and, in fact, can be used as an heuristic argument for the absence of long-range order at $T = 0$, just by using the Mermin-Wagner Theorem for classical systems at finite temperature.

4.2.8. What About the Excited States?

Up until now, we have been calling the AKLT model (as well as the MG model), an exactly solvable quantum spin model. However, this is strictly not true: all we could do was build the ground-state and, from it, take some rigorous conclusions about qualitative features of its spectrum. In other words, we cannot say anything about the nature of its low-energy excited states.

4.2.8.1. The Single-Mode Approximation

In this section, we will cope with this drawback by calculating an approximate expression for the Spin-Wave excitations over the AKLT ground-state. We will define and use the Single-Mode Approximation (SMA) invented by R. P. Feynman and D. Bijl to calculate the excitation spectrum above a condensate state of interacting bosons (an Helium-4 superfluid).

This technique relies on the assumption that the excited states of the system are obtained by acting on the exact ground-state, with the magnetization operator. Since this system is invariant under lattice translations, the eigenstates of H_{AKLT} can be labeled by a momentum quantum number - $q \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right[$, hence the SMA excited states are written as:

$$|q, \alpha\rangle = S_q^\alpha |AKLT\rangle, \quad for\ \alpha = x, y, z \tag{4.160}$$

Where the operator S_q^α is defined as in the Appendix 0A - $S_q^\alpha = \frac{1}{N}\sum_q S_n^\alpha e^{-iqan}$.

The energy associated with the state $|q, \alpha\rangle$ can also be obtained using the next expression[32]:

$$\Delta E_q^\alpha = E_q^\alpha - E_0 = \frac{\langle q, \alpha| H_{AKLT} |q, \alpha\rangle}{\langle q, \alpha \mid q, \alpha\rangle} - E_0 = \frac{1}{2}\frac{\langle AKLT| \left[S_{-q}^\alpha, \left[H_{AKLT}, S_q^\alpha\right]\right] |AKLT\rangle}{\langle AKLT| S_{-q}^\alpha S_q^\alpha |AKLT\rangle} \tag{4.161}$$

[31] Remember that the Haldane Mapping that we have found in Ch. 3, mapped a D-dimensional quantum system, to a classical $D+1$-dimensional one.

[32] Notice that $\left[S_{-q}^\alpha, \left[H_{AKLT}, S_q^\alpha\right]\right] = S_{-q}^\alpha H_{AKLT} S_q^\alpha + S_q^\alpha H_{AKLT} S_{-q}^\alpha - S_{-q}^\alpha S_q^\alpha H_{AKLT} - H_{AKLT} S_{-q}^\alpha S_q^\alpha$. Taking the expectation value of this in $|AKLT\rangle$ yields the following:

$$\langle AKLT| \left[S_{-q}^\alpha, \left[H_{AKLT}, S_q^\alpha\right]\right] |AKLT\rangle = \langle AKLT| S_{-q}^\alpha S_q^\alpha |AKLT\rangle \{E_q + E_{-q} - 2E_0\}$$

Finally, by using the inversion symmetry of the lattice, one may assume $E_q = E_{-q}$, giving the wanted result.

4.2.8.2. The SMA Dispersion Relation for the AKLT Model

References: [33]

Equation (4.160) is only useful to obtain the dispersion relation for these excitations, if we are able to calculate the numerator and the denominator. We can start by interpreting the quantity $S_{AKLT}(q) = \langle AKLT| S^{\alpha}_{-q} S^{\alpha}_{q} |AKLT\rangle$, as follows:

$$S_{AKLT}(q) = \frac{1}{N^2}\sum_{n,m}\langle AKLT| S^{\alpha}_{n} S^{\alpha}_{m} |AKLT\rangle e^{-iqa(n-m)} = \frac{1}{N^2}\sum_{n}\sum_{r}\langle AKLT| S^{\alpha}_{0} S^{\alpha}_{r} |AKLT\rangle e^{-iqar} = \\ = \frac{1}{N}\sum_{r}\langle AKLT| S^{\alpha}_{0} S^{\alpha}_{r} |AKLT\rangle e^{-iqar} \tag{4.162}$$

To obtain the equation (4.161), we have used the translation invariance of the system. In the end, this result allows us to interpret $S_{AKLT}(q)$ as the Fourier transform of the spin-spin correlation function in the AKLT ground-state. This we can calculate precisely as follows[33]:

$$S_{AKLT}(q) = \frac{2}{3N} + \frac{1}{N}\frac{4}{3}\sum_{r=-\infty(\neq 0)}^{\infty}(-1)^r 3^{-|r|} e^{-iqar} = \frac{2}{3N}\left[1 + 4Re\left\{\sum_{r=1}^{\infty} e^{-(\ln 3 + iqa + i\pi)r}\right\}\right] \Rightarrow \tag{4.163}$$

$$\Rightarrow S_{AKLT}(q) = \frac{2}{N}\frac{1-\cos qa}{5+3\cos qa} \tag{4.164}$$

Similarly, the double commutator can also be calculated explicitly [Appendix D.5], yielding the following result:

$$\langle AKLT|\left[S^{\alpha}_{-q},\left[H_{AKLT}, S^{\alpha}_{q}\right]\right]|AKLT\rangle = \frac{4J}{3N^2}\sum_{j\in\mathscr{L}}\left\langle\left(S^{x}_{j}S^{y}_{j+1} - S^{y}_{j}S^{x}_{j+1}\right)^2\right\rangle[1-\cos qa] \tag{4.165}$$

Now, we can use the expression (4.160) and plug in the results (4.163) and (4.164), to obtain the final expression for the dispersion relation:

$$\Delta E^{\alpha}_{q} = \frac{1}{2}\frac{\langle AKLT|\left[S^{\alpha}_{-q},\left[H_{AKLT}, S^{\alpha}_{q}\right]\right]|AKLT\rangle}{S_{AKLT}(q)} = \frac{J}{N}\sum_{j}\left\langle\left(S^{x}_{j}S^{y}_{j+1} - S^{y}_{j}S^{x}_{j+1}\right)^2\right\rangle\{5/3 + \cos qa\} = \\ = \frac{5J}{9}\{5/3 + \cos qa\} \tag{4.166}$$

The last equality is a result that we were not able to obtain, although it is stated in [33]. Nevertheless, the conclusion that there is a finite gap above the ground-state, does not depend of the precise value of the average in (4.165).

[33] Where we have used the summation formula for the geometric series - $\sum_{i=1}^{+\infty} r^i = \frac{r}{1-r}$.

The plot of this dispersion relation (in the FBZ of the chain) is shown in [Figure 4.8] where it is clear the existence of a gap located at the edge of the FBZ, with a value $\Delta_{SMA} = {}^{10J}/_{27} \simeq 0.370J$. This is nothing but the gap we expected for the AKLT model, that we proved rigorously before. The estimated value is in good agreement with numerical studies, as accounted in [33].

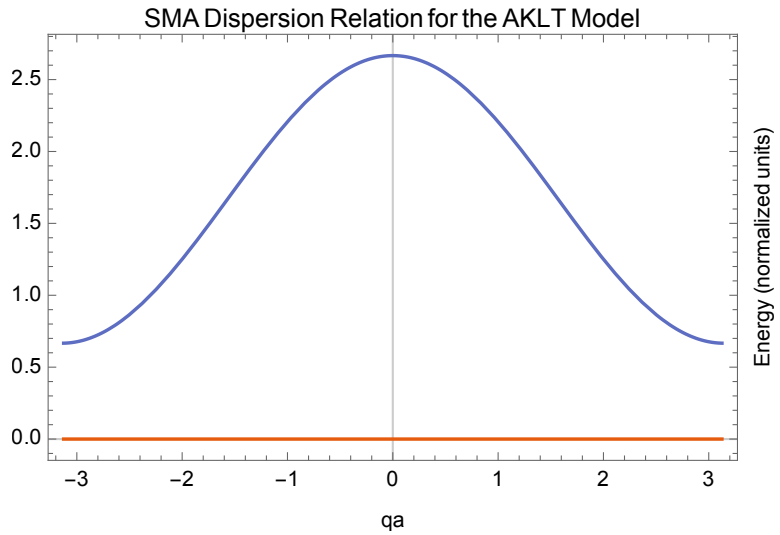


Figure 4.8.: Plot of the SMA dispersion relation for the whole FBZ of the chain. In the horizontal axis we have the reduced crystal momentum - qa - and in the vertical, we have the excitation energy, in units of ${}^{5}/_{9}J$.

4.3. Generalizations of the VBS State

References: [33,34]

4.3.1. The AKLT Construction In An Arbitrary Lattice

Already in the original articles by AKLT [31,32], it was recognized that the construction of a VBS state should be possible in any lattice, as long as the local spin multiplicity s is chosen accordingly. In fact, it is possible to take any lattice with coordination number $z$containing local spins $s = {}^{1}/_{2}J_M z$, and perform exactly the same kind of contraction to ensure that, for each nearest-neighbor bond, there will be no spin projection larger or equal than J_M. This procedure will involve 'breaking' the local spins into z virtual spins-${}^{1}/_{2}$ and then contracting each one into singlets with the corresponding spins of the first neighbors. Since the number of neighbors is also z, there will be no uncontracted virtual spins in any site of the bulk.

The resulting VBS state can be easily represented graphically (as depicted in the [Figure 4.9] for three cases), but using the index notation of this chapter or the product basis would yield incredibly complicated expressions. The main reason for this is the fact that the local states must still belong to the s multiplet and finding the general form for the $s$states in terms of the $z$virtual spin-${}^{1}/_{2}$ is not easy in the general case (as it was for the $s = 1$.)

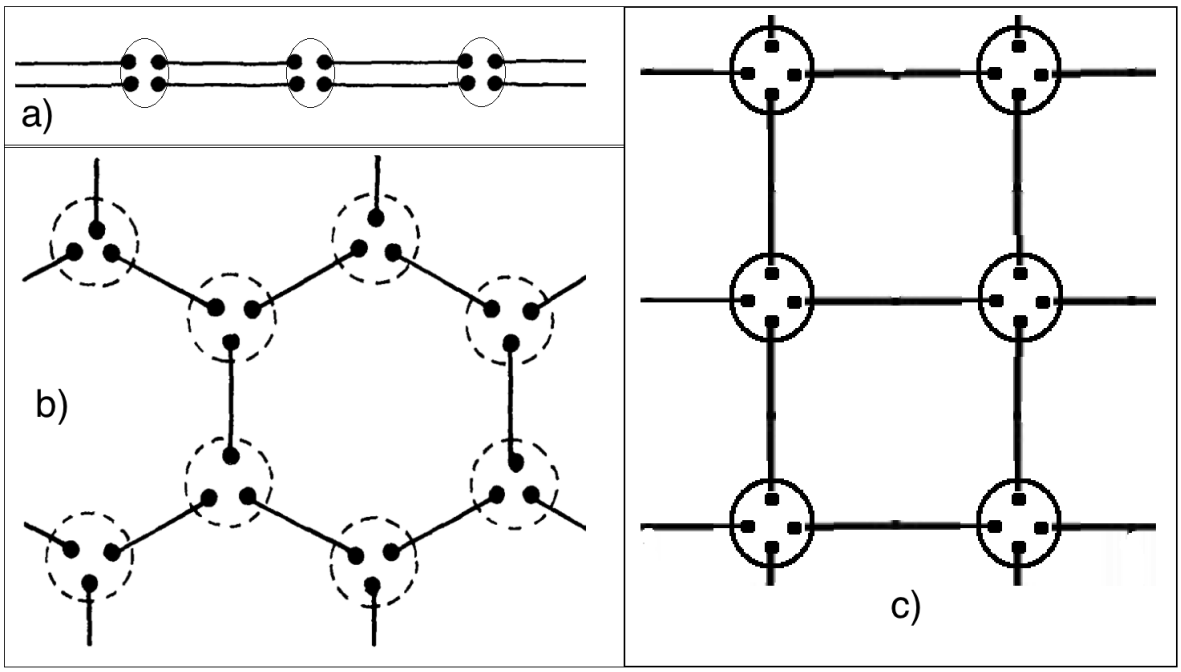


Figure 4.9.: a) The double valence-bond AKLT state in the one-dimensional chain with $s = 2$; b) The two-dimensional AKLT state in the Honeycomb lattice with $s = 3/2$; c) The two-dimensional AKLT state in the square lattice with $s = 2$.

However, we can use the representation of Subsection 4.2.4 to write these generalized VBS states, as follows[34]:

$$|VBS, J_M\rangle = \prod_{\langle i,j\rangle \in \mathscr{L}} \left(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger\right)^{J_M} |\omega\rangle \tag{4.167}$$

Clearly the state (4.166) yield the correct local spin quantum numbers, since each of the terms will have zJ_M creation operators of both types, associated to each individual site in $\mathscr{L}$[35]. These states can also be represented in terms of the spin coherent basis, yielding a wavefunction of the following form:

$$\begin{aligned}\Psi^N_{VBS}(\hat{\Omega}, J_M) = \left\langle VBS, J_M \mid \hat{\Omega}\right\rangle^* = \langle\omega| \prod_{\langle i,j\rangle \in \mathscr{L}} \left(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger\right)^{J_M} \prod_{i\in\mathscr{L}} \frac{\left(u_i a_i^\dagger + v_i b_i^\dagger\right)^{2s}}{\sqrt{(2s)!}} |\omega\rangle^* \Rightarrow \\ \Psi^N_{AKLT}(\hat{\Omega}) = (2J_M!)^N \prod_{\langle i,j\rangle \in \mathscr{L}} \left(u_i^* v_j^* - u_j^* v_i^*\right)^{J_M}\end{aligned} \tag{4.168}$$

Where $u_i(\theta_i, \phi_i) = e^{-i\phi_i/2}\cos\theta_i/2$ and $v_i(\theta_i, \phi_i) = e^{i\phi_i/2}\sin\theta_i/2)$, as usual. The modulus-square of the wavefunction has a very similar form to the one we have obtained in the AKLT case, i.e:

[34] This is for the case of the infinite lattice. If one wants to impose boundary conditions, we must proceed like in the AKLT case.

[35] Remember that, in the Schwinger Boson formalism, one has $J = 1/2(n_a + n_b)$.

$$\left|\Psi^N_{AKLT}(\hat{\Omega})\right|^2 = (2J_M!)^N \prod_{\langle i,j\rangle\in\mathscr{L}} \left(\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_j}{2}\right)^{J_M} \tag{4.169}$$

Finally, all the observables associated with this state can be calculated as before, using the diagonal representations of these operators in terms of coherent states, and then integrating it with the weight (4.168) over all the parameters. Obviously, the clever trick we have used for calculating the spin-spin correlation function in the AKLT state will not hold for an arbitrary state although, according to [33,34], it should hold for all the one-dimensional VBS states.

4.3.2. The Parent Hamiltonian of a VBS state

References: [7, 32, 34]

We have been able to generalize the VBS state to any lattice of spins, but still not established if these are ground-states of local Hamiltonians. In a sense, we have provided the answer before asking the question. Still, it is obvious what we must do to find the Hamiltonian whose exact ground-state will be the VBS state — $|VBS, J_M\rangle$. Any Hamiltonian involving only first-neighbor terms that are linear combinations of projectors $P_k(i,j)$ for $k \in \{J_M, ..., 2s\}$, will necessarily do the job, i.e.:

$$H_{VBS} = \sum_{\langle i,j\rangle\in\mathscr{L}} \left[\sum_{k=J_M}^{2s} V_k P_k(i,j)\right] \quad for \quad any \quad V_k \in \mathbb{R} \tag{4.170}$$

This last Hamiltonian is called a **Parent Hamiltonian** for the state $|VBS, J_M\rangle$, since $H_{VBS}\,|VBS, J_M\rangle = 0$. If we wish to express (4.169) in terms of spin coupling terms, we just have to generalize our procedure used in building the bond spin projectors for the AKLT hamiltonian. This allow us to write the following general expression:

$$P_k(i,j) = \prod_{\substack{n=0\\(n\neq k)}}^{2s} \left[\frac{\left(\vec{\mathbf{S}}_i + \vec{\mathbf{S}}_j\right)^2 - n(n+1)}{k(k+1) - n(n+1)}\right] = \prod_{\substack{n=0\\(n\neq k)}}^{2s} \left[\frac{2\left(\vec{\mathbf{S}}_i\cdot\vec{\mathbf{S}}_j\right) + 2s(s+1) - n(n+1)}{k(k+1) - n(n+1)}\right] \tag{4.171}$$

The form (4.170) is easily justified by noticing that, for each of the terms in the product, one has:

$$\left[\frac{\left(\vec{\mathbf{S}}_i + \vec{\mathbf{S}}_j\right)^2 - n(n+1)}{k(k+1) - n(n+1)}\right] |k,m\rangle = \frac{k(k+1) - n(n+1)}{k(k+1) - n(n+1)}\,|k,m\rangle = |k,m\rangle \tag{4.172}$$

Finally, from (4.170) we see that a VBS state with maximum bond spin J_M is the exact ground-state of an AFM Hamiltonian with only first-neighbor spin interactions, that are polynomials $P\left(\vec{\mathbf{S}}_i\cdot\vec{\mathbf{S}}_j\right)$

of degree zJ_M. To exemplify all of this construction, we list the ground-states and the corresponding Parent Hamiltonians[36] for the three examples shown in [Figure 4.9.]:

- Spin-2 AKLT Chain:

$$\left|AKLT^2\right\rangle = \prod_{k=-\infty}^{\infty} \left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)^2 |\omega\rangle \tag{4.173}$$

$$H_{AKLT^2} = K \sum_{i=-\infty}^{\infty} \left\{ \left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right) + \frac{327}{1522}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right)^2 + \right.$$
$$\left. + \frac{15}{761}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right)^3 + \frac{1}{1522}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1}\right)^4 \right\}, \quad K > 0 \tag{4.174}$$

- Spin-3/2 VBS in the Honeycomb Lattice:

$$|VBS_{Honeycomb}\rangle = \prod_{\langle i,j\rangle} \left(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger\right) |\omega\rangle \tag{4.175}$$

$$H_{Honeycomb}^{VBS} = K \sum_{\langle i,j\rangle} \left\{ \left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right) + \frac{116}{243}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right)^2 + \frac{16}{243}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right)^3 \right\}, \quad K > 0 \tag{4.176}$$

- Spin-2 VBS state in the Honeycomb Lattice:

$$|VBS_{Square}\rangle = \prod_{\langle i,j\rangle \in \mathscr{L}} \left(a_i^\dagger b_j^\dagger - a_j^\dagger b_i^\dagger\right) |\omega\rangle \tag{4.177}$$

$$H_{Square}^{VBS} = K \sum_{\langle i,j\rangle \in \mathscr{L}} \left\{ \left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right) + \frac{327}{1522}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right)^2 + \right.$$
$$\left. + \frac{15}{761}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right)^3 + \frac{1}{1522}\left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_j\right)^4 \right\}, \quad K > 0 \tag{4.178}$$

All these Hamiltonians are altered versions of the usual first-neighbor Heisenberg AFM model, in the respective lattices.

4.3.3. VBS Heuristics

References: [33,34]

In Chapter 3, it has been proved that the usual Heisenberg AFM model in a D-dimensional lattice at $T = 0$ can be mapped into a classical model in $(D + 1)$-dimensional at a finite temperature. This is a very general statement about quantum models, since the building of the partition function will always involve an integration in imaginary time, plus the usual summation over all the lattice points.

In the case of the VBS models, the ground-state physics (i.e $T = 0$) can also be mapped onto a classical model. This is done (as in section 4.2.7) by using the coherent state basis, where any local observable

[36] Notice that the parent Hamiltonians for a given VBS state are not unique. However, the degree of the polynomial 2-spin interaction is always the same, independently of the choice.

can be represented by a function - $\mathcal{A}(\hat{\Omega})$ - and the corresponding expectation values in the ground-state can be written as follows:

$$\langle A\rangle_{VBS} = \frac{\int d\Omega \mathscr{A}(\Omega)\left|\Psi^N_{AKLT}(\Omega)\right|^2}{\int d\Omega \left|\Psi^N_{AKLT}(\Omega)\right|^2} = \frac{\int d\Omega \mathscr{A}(\Omega)\exp\left[-J_M\sum_{\langle i,j\rangle\in\mathscr{L}}\left(\ln\left\{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}\right\}^{-1}\right)\right]}{\int d\Omega \exp\left[-J_M\sum_{\langle i,j\rangle\in\mathscr{L}}\left(\ln\left\{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}\right\}^{-1}\right)\right]} \tag{4.179}$$

In this logic, we can associate to the $T=0$ VBS state, a classical partition function given as:

$$Z_{J_M} = \int d\Omega \exp\left[-J_M\sum_{\langle i,j\rangle\in\mathscr{L}}\left(\ln\left\{1-\hat{\Omega}_i\cdot\hat{\Omega}_{i+1}\right\}^{-1}\right)\right] \tag{4.180}$$

This result is rather surprising, since (4.179) is the canonical partition function of a D-dimensional system of classical spins, with first-neighbor interactions. An immediate consequence of this is that the spin-spin correlation functions for $D=1,2$ are exponentially decaying, and the states thus disordered. This fact is proven rigorously in [32] for the honeycomb lattice.

4.4. Summary

In this chapter, we explored two one-dimensional quantum spin models, for which the exact ground-state can be found. In both cases, we have proved rigorously that the systems are gapped in the thermodynamic limit, and the corresponding ground-states have only short-ranged correlations among the spins. The construction of the ground-states allowed for the definition of two interesting types of quantum states — the Resonating Valence-Bond State (RVB) and also the Valence-Bond Solid State (VBS) — and the former was then generalized for any lattice beyond the one-dimensional chain.

The study of both these models interested us for two reasons: First of all, because they are intimately related with the Heisenberg Model, which we have been exploring form the first 3 chapters. And secondly, because the construction of these ground-states actually laid the foundations for the development of powerful numerical methods that allow for a more efficient study of large interacting quantum systems, using variational methods. This point of view will be briefly introduced in the next chapter.

5. Tensor Product States and Conclusions

Last chapter, we have explored the MG and AKLT one-dimensional models, mainly because their ground-states and low-energy properties were known exactly, but also because they were closely related to the Heisenberg Model. However, the process of building these exact ground-states revealed to be interesting in its own right, helping to define a new class of quantum manybody states. This class of states, as we will see, are useful in describing real spin systems and, in particular seem to capture the essential physical features of the Heisenberg AFM.

In this last chapter, we will see how to use of the AKLT procedure for defining a new class of quantum states, associated to an one-dimensional chain of quantum spins — the **Matrix Product States** (MPS). These complex states can be shown to obey an **area law of entanglement**, which seems to be an essential feature of the ground-states of gapped models with local Hamiltonians [35]. This is precisely the case of the Heisenberg AFM chain, with integer local spins, as conjectured in chapter 3.

5.1. The Abstract MPS Construction

5.1.1. Motivation

To build a MPS, we must generalize the original AKLT construction (Section 4.2) and consider a chain of abstract local quantum systems, whose Hilbert Spaces — $\mathscr{H}_s^d$ — are d-dimensional. In this case, the complete Hilbert Space for the whole system will be the tensor product — $\mathscr{H}_{Tot(N)} = \otimes_{s\in\mathscr{L}}\mathscr{H}_s^d$ — and any state can be represented as follows:

$$\left|\varphi^N\right\rangle = \sum_{i_1,\ldots,i_N=0}^{d} C_{i_1\ldots i_N} \left|i_1\right\rangle \otimes \ldots. \otimes \left|i_N\right\rangle \tag{5.1}$$

Then a general state of the system can be fully defined by a total of $d^{N-1}-1$ independent complex parameters. Working with such a representation is impracticable, if the number of sites is realistically large. Furthermore, we know that most of the states in the class (5.1) simply do not show up as low-energy states for systems described by local Hamiltonians, because they do not exhibit the correct entanglement properties. Hence, we can inspire ourselves in the AKLT construction to find a better (and more restricted) class of states, that can be valid ground-states of these local systems, and this will be the subject of the remaining discussion.

5.1.2. The MPS Construction

References: [35]

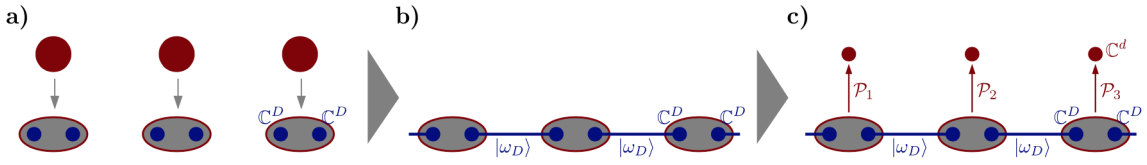


Figure 5.1.: Representation of the 3 steps taken for constructing a Matrix Product State.

The first step we may take, is to replace the local d-dimensional systems, by a pair of virtual D-dimensional identical systems, with an Hilbert Space — $\mathscr{H}_s^D \otimes \mathscr{H}_s^D$. This dimension D need not have any particular relation with the dimensionality of the original local systems. This step is represented in Figure 5.1 a).

Secondly, we can do something similar to the AKLT construction, and impose that a virtual system in a given site, is in a maximally entangled state (a generalized Bell state), with one of the virtual systems of the neighboring site. This **Bond State** is written in the space — $\mathscr{H}_s^D \otimes \mathscr{H}_{s+1}^D$ — as follows[1]:

$$|\omega_D\rangle_s^{s+1} \equiv \frac{1}{\sqrt{D}} \sum_{\alpha=1}^{D} |\alpha\rangle_{(s,2)} \otimes |\alpha\rangle_{(s+1,1)} \tag{5.2}$$

The state (5.2) can now be generalized to the whole chain. Considering a finite chain with N sites, we have the following manybody wavefunction:

$$\left|\Theta_{\alpha\beta}^N\right\rangle = |\alpha\rangle_{(1,1)} \otimes \left[\otimes_{s=1}^N |\omega_D\rangle_s^{s+1}\right] \otimes |\beta\rangle_{(N,1)} \tag{5.3}$$

Note that the edge degrees of freedom remain free in this formalism, and are represented by the indices $\alpha, \beta = \{1, ..., D\}$.

The states (5.3) seem to be a very uninteresting set of product states, that do not approach the complexity expected for the MPS. However, these are not states of the original lattice, but instead of the lattice of virtual D-level systems. In order to return to the original description, we must project the local virtual states — in $\mathscr{H}_s^D \otimes \mathscr{H}_s^D$ — into the **physical subspace** — $\mathscr{H}_s^d$.

This is done by applying a **local linear transformation** — represented by the operator $\mathcal{P}_s$, as follows:

$$\begin{aligned} \mathcal{P}_s : \quad \mathscr{H}_s^D \otimes \mathscr{H}_s^D \quad &\rightarrow \quad \mathscr{H}_s^d \\ |\alpha\rangle_{(s,1)} \otimes |\beta\rangle_{(s,2)} \quad &\rightarrow \quad \sum_{i=0}^{d} M_{i,\alpha\beta}^{[s]} |i\rangle_s \end{aligned} \tag{5.4}$$

Or in a simplified braket notation:

[1]The notation used in (5.2) labels the state α of the virtual system $k = 1, 2$ associated to the site i, by the ket $|\alpha\rangle_{(i,k)}$.

$$\mathcal{P}_s = \sum_{\alpha,\beta=0}^{D} \sum_{i=0}^{d} M_{i,\alpha\beta}^{[s]} \left|i\right\rangle \left\langle \alpha,\beta\right| \tag{5.5}$$

In (5.4), the set of numbers $M_{i,\alpha\beta}^{[s]}$ are the coefficients of the tensor that represents $\mathcal{P}_s$ in the basis $\left|i\right\rangle \left\langle \alpha,\beta\right|$. The final MPS is obtained by applying (5.4) in each site, to the state (5.3). This yields:

$$\left|\Psi_{\alpha\beta}^{N}\right\rangle = \left[\mathcal{P}_1 \otimes ... \otimes \mathcal{P}_N\right] \left|\Theta_{\alpha\beta}^{N}\right\rangle \tag{5.6}$$

It is interesting to see how does the state (5.6) look in terms of the product states of $\mathscr{H}_{Tot(N)}$. The coefficients can be written in terms of the matrices — $M_{i,\alpha\beta}^{[s]}$ — which can be seen by calculating the action of the projectors in (5.6). For that, we must deal separately with the projection for the bulk states and the edges, i.e.:

- **Bulk Projections** (sites s and $s+1$):

$$\begin{aligned}
\left[\mathcal{P}_s \otimes \mathcal{P}_{s+1}\right] \left|\Theta_{\alpha\beta}^{N}\right\rangle &= \left[\mathcal{P}_s \otimes \mathcal{P}_{s+1}\right] \left[... \otimes \left|\omega_D\right\rangle_{s-1}^{s} \otimes \left|\omega_D\right\rangle_{s}^{s+1} \otimes \left|\omega_D\right\rangle_{s+1}^{s+2} \otimes ...\right] = \\
&= \frac{1}{D^{3/2}} \left[\mathcal{P}_s \otimes \mathcal{P}_{s+1}\right] \left[... \otimes \sum_{\alpha\beta\gamma=0}^{D} \left|\alpha,\alpha,\beta,\beta,\gamma,\gamma\right\rangle \otimes ...\right] = \\
&= \frac{1}{D^{3/2}} \left[... \sum_{\alpha\beta\gamma=0}^{D} \left|\alpha\right\rangle \otimes \left\{\mathcal{P}_s \left|\alpha,\beta\right\rangle\right\} \otimes \left\{\mathcal{P}_{s+1} \left|\beta,\gamma\right\rangle\right\} \otimes \left|\gamma\right\rangle ...\right]
\end{aligned} \tag{5.7}$$

Now, we can use the definition (5.5) for the projectors and calculate the single-site action expressed in (5.7). This goes as follows:

$$\begin{aligned}
&... \sum_{\alpha\beta\gamma=1}^{D} \left|\alpha\right\rangle \otimes \left[\sum_{i=1}^{d} \sum_{\alpha_1\beta_1=1}^{D} M_{i,\alpha_1\beta_1}^{[s]} \left|i\right\rangle \left\langle \alpha_1,\beta_1 \mid \alpha,\beta\right\rangle\right] \otimes \\
&\qquad \otimes \left[\sum_{j=1}^{d} \sum_{\alpha_2\beta_2=1}^{D} M_{j,\alpha_2\beta_2}^{[s+1]} \left|j\right\rangle \left\langle \alpha_2,\beta_2 \mid \beta,\gamma\right\rangle\right] \otimes \left|\gamma\right\rangle ... = \\
&= ... \sum_{\alpha\beta\gamma=1}^{D} \left|\alpha\right\rangle \otimes \left[\sum_{i=1}^{d} M_{i,\alpha\beta}^{[s]} \left|i\right\rangle\right] \otimes \left[\sum_{j=1}^{d} M_{j,\beta\gamma}^{[s+1]} \left|j\right\rangle\right] \otimes \left|\gamma\right\rangle ... = \\
&= ... \sum_{\alpha\gamma=1}^{D} \left|\alpha\right\rangle \otimes \left[\sum_{i,j,\beta} M_{i,\alpha\beta}^{[s]} M_{j,\beta\gamma}^{[s+1]} \left|i\right\rangle \otimes \left|j\right\rangle\right] \otimes \left|\gamma\right\rangle ... = \\
&= ... \sum_{\alpha\gamma=1}^{D} \left|\alpha\right\rangle \otimes \left[\sum_{i,j=1}^{d} \left[\mathbb{M}_i^{[s]} \cdot \mathbb{M}_j^{[s+1]}\right]_{\alpha\gamma} \left|i\right\rangle \otimes \left|j\right\rangle\right] \otimes \left|\gamma\right\rangle ...
\end{aligned} \tag{5.8}$$

And in (5.8), we have defined — $\mathbb{M}_i^{[s]}$ — as being $D \times D$ matrices with elements $\left[\mathbb{M}_i^{[s]}\right]_{\alpha\beta} \equiv M_{i,\alpha\beta}^{[s]}$.

- **Edge Projections** (sites 1 and N):

$$\begin{aligned}
[\mathcal{P}_1 \otimes \mathcal{P}_2] \left|\Theta^N_{\alpha\beta}\right\rangle &= [\mathcal{P}_1 \otimes \mathcal{P}_2] \left[|\alpha\rangle \otimes |\omega_D\rangle_1^2 \otimes |\omega_D\rangle_2^3 \otimes ...\right] = \\
&= \frac{1}{D} [\mathcal{P}_1 \otimes \mathcal{P}_2] \left[... \otimes \sum_{\beta\gamma=0}^{D} |\alpha, \beta, \beta, \gamma, \gamma\rangle \otimes ...\right] = \\
&= \frac{1}{D} \left[... \sum_{\beta\gamma=0}^{D} \{\mathcal{P}_1 |\alpha, \beta\rangle\} \otimes \{\mathcal{P}_2 |\beta, \gamma\rangle\} \otimes |\gamma\rangle ...\right]
\end{aligned} \tag{5.9}$$

Once again, by using the definition (5.6) for the local projectors, we can calculate (5.9) as follows:

$$\begin{aligned}
&\sum_{\beta\gamma=1}^{D} \left[\sum_{i=1}^{d} \sum_{\alpha_1\beta_1=1}^{D} M^{[s]}_{i,\alpha_1\beta_1} |i\rangle \langle\alpha_1, \beta_1 \mid \alpha, \beta\rangle\right] \otimes \\
\otimes \left[\sum_{j=1}^{d} \sum_{\alpha_2\beta_2=1}^{D} M^{[s+1]}_{j,\alpha_2\beta_2} |j\rangle \langle\alpha_2, \beta_2 \mid \beta, \gamma\rangle\right] \otimes |\gamma\rangle ... &= \sum_{\beta\gamma=1}^{D} \left[\sum_{i=1}^{d} M^{[s]}_{i,\alpha\beta} |i\rangle\right] \otimes \left[\sum_{j=1}^{d} M^{[s+1]}_{j,\beta\gamma} |j\rangle\right] \otimes |\gamma\rangle = \\
= \sum_{\alpha,\gamma=1}^{D} \left[\sum_{i,j,\beta} M^{[s]}_{i,\alpha\beta} M^{[s+1]}_{j,\beta\gamma} |i\rangle \otimes |j\rangle\right] \otimes |\gamma\rangle ... &= \sum_{\gamma=1}^{D} \left[\sum_{i,j=1}^{d} \left[\mathbb{M}^{[s]}_i \cdot \mathbb{M}^{[s+1]}_j\right]_{\alpha\gamma} |i\rangle \otimes |j\rangle\right] \otimes |\gamma\rangle ...
\end{aligned} \tag{5.10}$$

Considering equations (5.8) and (5.10), we conclude that the states — $\left|\Psi^N_{\alpha\beta}\right\rangle$ — can be written as:

$$\left|\Psi^N_{\alpha\beta}\right\rangle = \sum_{i_1,...,i_N=1}^{d} \left[\mathbb{M}^{[1]}_{i_1} \cdot \mathbb{M}^{[2]}_{i_2} ... \cdot \mathbb{M}^{[N-1]}_{i_{N-1}} \cdot \mathbb{M}^{[N]}_{i_N}\right]_{\alpha\beta} |i_1\rangle \otimes .... \otimes |i_N\rangle \tag{5.11}$$

Or, by imposing Periodic Boundary Conditions (PBC), we see that (5.11) turns into the following:

$$\left|\Psi^N_{PBC}\right\rangle = \sum_{\alpha=1}^{D} \left|\Psi^N_{\alpha\alpha}\right\rangle = \sum_{i_1,...,i_N=1}^{d} Tr\left[\mathbb{M}^{[1]}_{i_1} \cdot \mathbb{M}^{[2]}_{i_2} ... \cdot \mathbb{M}^{[N-1]}_{i_{N-1}} \cdot \mathbb{M}^{[N]}_{i_N}\right] |i_1\rangle \otimes .... \otimes |i_N\rangle \tag{5.12}$$

The states (5.11) and (5.12) are called **Matrix Product States** (MPS), since their coefficients (in the product state representation) are written as products of matrices.

5.1.3. The Matrix Product States as an Efficient Variational Class

References: [35]

At first sight, it is not clear why the MPS class may be useful in any way, since ultimately we describe these states in terms of the product basis. However, this conclusion is naive, since we see that there are only D^2 independent parameters in each matrix and we need at most $N \times d$ different matrices to describe a state like (5.11). In addition to this, if we impose extra symmetries in the states — e.g.

translational symmetry — the matrices are site-independent and the total number of free parameters decreases to just $d \times D$. In other words, the MPS represent only a small corner of the Hilbert Space for the whole chain, but is still able to capture the the physically significant states for describing the low-energy physics of local Hamiltonians.

An important use for this restricted class of quantum states, is the determination of approximate ground-states for local quantum Hamiltonians, like — $H^N_{system} = \sum_i H_i$. This can be done by using variational techniques, in which the state of the system is assumed to belong to a class $|\phi(\lambda_1, ...)\rangle$ depending on a number of free parameters — $\{\lambda_i\}_i$. Inside this class of states, the expectation value of the energy is calculated as a function of these same parameters, yielding the following:

$$\langle E\rangle_\phi (\lambda_1, ...) = \frac{\langle\phi(\lambda_1, ...)| H^N_{system} |\phi(\lambda_1, ...)\rangle}{\langle\phi(\lambda_1, ...) \mid \phi(\lambda_1, ...)\rangle} = f_\phi(\lambda_1, ...) \tag{5.13}$$

The approximate ground-state for H^N_{system} is the one that minimizes the function f_ϕ in (5.13). Obviously, the quality of this approximation will improve, if we consider ever larger classes of states in $\mathscr{H}_{Tot(N)}$, and it will be exact if the variational parameters are the coefficients of the state (5.1). However, the larger the number of parameters, the slower will the method converge to the minimum value. Hence, if we want to deal with macroscopic systems, using the general state (5.1) as a variational class would be computationally impractical. This is the point where the states (5.11) and (5.12) become useful.

As discussed in the ref. [35], the calculation of the averages (5.13), can be done efficiently inside the MPS class and the number of variational parameters grows only linearly with the number of sites[2]. Therefore, the MPS states (and its generalizations to higher-dimensions — the **Tensor Product States**) represent a set of important states to study interacting quantum systems, using numerical techniques.

5.1.4. The AKLT and MG Models as Examples of MPS

To conclude this short discussion, we will show how to write the ground-states of the one-dimensional AKLT model and the Majumdar-Ghosh model in the MPS formalism. In fact, both of these models are examples of gapped spin hamiltonians in which the exact ground-states are found to be Matrix Product States, which is supposed to be a general result.

The AKLT Ground-State:

Starting with the AKLT model, we can see that the dimension of the original local spaces is $d = 3$ (a triplet of states), while the virtual ones have $D = 2$. As a convention, we will define the following basis for each of these spaces, as follows:

[2] Assuming translation invariance, the number of parameters is even independent of N. However, for a good convergence one may need to increase the bond dimension — D — with the number of sites. [35]

$$\mathscr{H}_s^{d=3} = Span\left\{|+\rangle, |0\rangle, |-\rangle\right\} \tag{5.14}$$
$$\mathscr{H}_{s,1}^{D=2} = Span\left\{|\uparrow\rangle, |\downarrow\rangle\right\} \tag{5.15}$$
$$\mathscr{H}_{s,2}^{D=2} = Span\left\{|\downarrow\rangle, -|\uparrow\rangle\right\} \tag{5.16}$$

The different choices of basis in (5.15) and (5.16) is done such that the bond states defined in (5.2), are singlets of spin. We have done this choice implicitly in Section 4.2., when we defined the lifting of indexes using the antisymmetric tensor — $\epsilon^{\alpha\beta}$. By using these basis, the complete expression of the local projectors is given easily, as follows:

$$\mathcal{P}_{AKLT} = |+\rangle\langle\uparrow\uparrow| + \frac{1}{\sqrt{2}}|0\rangle\left\{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|\right\} + |-\rangle\langle\downarrow\downarrow| \tag{5.17}$$

The expression (5.16) is already written in the form (5.5), which translates into the following coefficient matrices:

$$\mathbb{M}_+ = \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix} \quad \mathbb{M}_0 = \begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{2} \end{bmatrix} \quad \mathbb{M}_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{5.18}$$

Hence, the (non-normalized) AKLT ground-state in the Periodic chain (the other cases are analogous), can be written as follows:

$$\left|AKLT_N^{PBC}\right\rangle = \sum_{i_1 \ldots i_N = (-,0,+)} Tr\left[\mathbb{M}_{i_1}^{[1]} \cdot \mathbb{M}_{i_2}^{[2]} \ldots \cdot \mathbb{M}_{i_{N-1}}^{[N-1]} \cdot \mathbb{M}_{i_N}^{[N]}\right] |i_1\rangle \otimes .... \otimes |i_N\rangle \tag{5.19}$$

Finally, from the matrices (5.18), it is possible to obtain all of the rules stated in Subsection 4.2.2., for the representation of the AKLT ground-state in terms of product states. For example, there are no components in (5.19) that have the combination — $(... + 00 + ...)$ — since:

$$\mathbb{M}_+ \cdot \mathbb{M}_0 \cdot \mathbb{M}_0 \cdot \mathbb{M}_+ = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

The Majumdar-Ghosh Ground-State:

The demonstration that the AKLT ground-state is a MPS was trivial, since the MPS class was defined, using it as an inspiration. A bit more surprising than that, is to learn that also one of the RVB ground-states of the Majumdar-Ghosh model — Φ^+ — can be represented as a Matrix Product State with $D = 3$ and $d = 2$. To obtain this description, we start by considering the case of a periodic chain with 4 sites. Because the state is translation invariant, determining the matrices for a 4 site chain, is enough. The non-normalized ground-state for a 4 sites with PBC is given as:

$$\Phi^+ = |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle - 2\,|\uparrow\downarrow\uparrow\downarrow\rangle - 2\,|\downarrow\uparrow\downarrow\uparrow\rangle \tag{5.20}$$

For this can, it can be seen by direct calculation, that the following choice of matrices work:

$$\mathbb{M}_{\uparrow} = \begin{bmatrix} 0 & i & 0 \\ 0 & 0 & -i \\ 0 & 0 & 0 \end{bmatrix} \quad \mathbb{M}_{\downarrow} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{5.21}$$

Which allow us to write Φ^+ in the following final form:

$$\Phi^+ = \sum_{i_1 ... i_N = \uparrow,\downarrow} Tr\left[\mathbb{M}_{i_1} \cdot \mathbb{M}_{i_2} ... \cdot \mathbb{M}_{i_{N-1}} \cdot \mathbb{M}_{i_N}\right] |i_1\rangle \otimes .... \otimes |i_N\rangle \tag{5.22}$$

So, the RVB state is also a MPS, despite its original construction did not involve introducing any virtual degrees of freedom — as in the AKLT case.

5.2. Conclusions

In this work, we have explored several paths for studying the physics of interacting quantum spin models. Starting from the Heisenberg model, we have developed the standard spin-wave theory in chapter 1 and we have seen that despite it works well for three-dimensional lattices, it yields a lot of ill-defined results when applied to lower-dimensional systems, at finite or even zero temperature.

In the second chapter, we explored the notion of magnetic order for these models and we have established that the divergences at finite temperatures are the consequence of a rigorous result that prevents the existence of any order for one- or two-dimensional lattices of spins. Furthermore, we have proven rigorously that the exact ground-state is unique and isotropic, and also that the Heisenberg Model is gapless in the case of half-integer localized spins.

In the third chapter, we have used a powerful field-theoretical formulation for the D-dimensional Heisenberg Model, to show that it can be described, at any temperature, by a non-linear effective QFT, called the $O(3)$-Non-Linear Sigma model, in $(D+1)$-dimensions. Using this mapping, we were able to conjecture that the Heisenberg Chain with integer local spins, must be gapped and magnetically disordered (Haldane Conjecture).

Finally, in the forth chapter, we have studied some related one-dimensional models, that allowed for the exact construction of their ground-states. Both of this models (MG and AKLT) were found to have only short-ranged correlations in the ground-state (spin-Peierls in the MG case and exponential for the AKLT) and a finite energy gap over it, that survives in the thermodynamic limit. These two cases highlighted the importance of the RVB and VBS states as good conceptual candidates for approximating the complex ground-states of the pure Heisenberg Models.

In this last chapter, we have taken advantage of the AKLT method to define a new class of variational states — the Matrix Product States — that seem to capture the complexity of the ground-states of local spin Hamiltonians, but is not too large, as to make any variational method impractical. These states can be used to study several interesting systems of quantum spins, being one-dimensional, higher-dimensional, and can even be generalized for applications to fermionic systems [35]. However, if we

are to choose an interesting problem to which these methods, could be applied, it will have to be the Haldane Chain [6], defined as follows:

$$H_{Hal}(\beta) = \sum_{i=-\infty}^{\infty} \overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} + \beta \left(\overrightarrow{\mathbf{S}}_i \cdot \overrightarrow{\mathbf{S}}_{i+1} \right)^2 \quad for \quad s = 1$$

This one-parameter class of Hamiltonians include two of the discussed models — The Heisenberg Model ($\beta = 0$) and the AKLT Model ($\beta = 1/3$). As we vary β, the low-energy physics of the system suffers some changes, however those changes will only be qualitatively important if, for example, there happens to be a closing of the energy gap or a change in the degeneracy of the ground-state. In other words, we may have a quantum phase transition (at $T = 0$) for some critical values of β.

As far as we know, between $\beta = 0$ and $\beta = 1/3$ there are no such quantum phase-transitions and thus, we say that our models belong to the same quantum phase — the Haldane Phase — which corresponds to a gapped quantum spin liquid. However, it is predicted that for $\beta_c = -1$, there is a phase transition to a dimerized-phase, where the order if of the spin-Peierls type and the translational symmetry is broken. These facts were not lengthly explored here, but an interesting discussion can be found in [6].

A. Appendix

A.1. Lattice Sums and Discrete Fourier Transforms

Since lattice sums and Fourier transforms are always a big pain in the neck which generate constant confusions in the definitions, we have decided to fix conventions and review the necessary results that will be useful in some places during this work.

We start by defining the vectors of a Bravais lattice $\mathscr{L}$ as being of the form $\mathbf{R} = n_i \mathbf{a}^i$ and the corresponding dual lattice $\mathscr{L}^*$ as being composed of the vectors $\mathbf{K} = l^i \mathbf{b}_i$, for $\mathbf{b}_i \cdot \mathbf{a}^j = 2\pi\delta_i^j$ and $n_i, l^i \in \mathbb{Z}$. For future purposes, it is interesting to consider the following d-dimensional Bravais lattice sum (with N cells, with Periodic Boundary Conditions):

$$\sum_{\vec{\mathbf{R}} \in \mathscr{L}} e^{i \vec{\mathbf{k}} \cdot \vec{\mathbf{R}}}$$

To perform this sum over the whole lattice, we can use the periodicity of the lattice, itself. Starting by calling — $\overrightarrow{\mathbf{L}}$ — to an arbitrary vector in $\mathscr{L}$, and noting the following identity:

$$\sum_{\vec{\mathbf{R}} \in \mathscr{L}} e^{i \vec{\mathbf{k}} \cdot \vec{\mathbf{R}}} = \sum_{\vec{\mathbf{R}} \in \mathscr{L}} e^{i \vec{\mathbf{k}} \cdot \left(\vec{\mathbf{R}} + \vec{\mathbf{L}}\right)} \tag{A.1}$$

Manipulating the identity (A.1), we get to the following result:

$$\sum_{\vec{\mathbf{R}} \in \mathscr{L}} e^{i \vec{\mathbf{k}} \cdot \vec{\mathbf{R}}} \left[1 - e^{i \vec{\mathbf{k}} \cdot \vec{\mathbf{L}}}\right] = 0 \quad \forall \overrightarrow{\mathbf{L}} \in \mathscr{L} \tag{A.2}$$

From (A.2), we can conclude two things:

1. If $e^{i \vec{\mathbf{k}} \cdot \vec{\mathbf{L}}} \neq 1$ for some vector $\overrightarrow{\mathbf{L}} \in \mathscr{L}$, then — $\sum_{\mathbf{R} \in \mathscr{L}} e^{i\mathbf{k}\cdot\mathbf{R}} = 0$. This will happen if and only if $\overrightarrow{\mathbf{k}}$ is not a vector of the dual lattice $\mathscr{L}^*$;
2. If $\overrightarrow{\mathbf{k}} \in \mathscr{L}^*$, then — $\sum_{\mathbf{R} \in \mathscr{L}} e^{i\mathbf{k}\cdot\mathbf{R}} = \sum_{\vec{\mathbf{R}} \in \mathscr{L}} = N$;

These two results can be now condensed into a single equation, as follows:

$$\sum_{\vec{\mathbf{R}} \in \mathscr{L}} e^{i \vec{\mathbf{k}} \cdot \vec{\mathbf{R}}} = N \sum_{\mathbf{K} \in \mathscr{L}^*} \delta_{\vec{\mathbf{k}}, \vec{\mathbf{K}}} \tag{A.3}$$

And this is the result we wanted. One of the useful applications of (A.3), is to define and invert the Lattice Fourier Transform of a function:

Discrete Fourier Transform of a Lattice Function:

A lattice function $g : \mathscr{L} \to A$ is a function that assigns a given value in the set A, to each point of the real lattice. For such a function, we can define its Fourier representation as:

$$g(\overrightarrow{\mathbf{R}}) = \sum_{\overrightarrow{\mathbf{k}} \in FBZ} g(\overrightarrow{\mathbf{k}}) e^{i\overrightarrow{\mathbf{R}}\cdot\overrightarrow{\mathbf{k}}} \to \frac{N v_{cell}}{(2\pi)^d} \int_{FBZ} d^d\overrightarrow{\mathbf{k}}\, g(\overrightarrow{\mathbf{k}}) e^{i\overrightarrow{\mathbf{R}}\cdot\overrightarrow{\mathbf{k}}}$$

The sum/integral is only over the First Brillouin Zone (FBZ), which is a consequence of the lattice periodicity of g. Now, we can use the last result of the previous subsection to invert the above equation, yielding the Fourier Transform of a lattice function:

$$\begin{aligned}\sum_{\overrightarrow{\mathbf{R}} \in \mathscr{L}} g(\overrightarrow{\mathbf{R}}) e^{-i\overrightarrow{\mathbf{R}}\cdot\overrightarrow{\mathbf{k}}_1} &= \sum_{k \in FBZ} g(\overrightarrow{\mathbf{k}}) \sum_{\overrightarrow{\mathbf{R}} \in \mathscr{L}} e^{i\overrightarrow{\mathbf{R}}\cdot(\overrightarrow{\mathbf{k}}-\overrightarrow{\mathbf{k}_1})} = N \sum_{\overrightarrow{\mathbf{k}} \in FBZ} g(\overrightarrow{\mathbf{k}}) \sum_{\overrightarrow{\mathbf{K}} \in \mathscr{L}^*} \delta_{\overrightarrow{\mathbf{k}}-\overrightarrow{\mathbf{k}}_1, \overrightarrow{\mathbf{K}}} \\ &= N \sum_{\overrightarrow{\mathbf{k}} \in FBZ} g(\overrightarrow{\mathbf{k}}) \delta_{\overrightarrow{\mathbf{k}}-\overrightarrow{\mathbf{k}}_1, \overrightarrow{\mathbf{0}}} = N g(\overrightarrow{\mathbf{k}}_1)\end{aligned}$$

Therefore, the Discrete Fourier Transform of a Lattice function is defined as:

$$g(\overrightarrow{\mathbf{k}}) = \frac{1}{N} \sum_{\overrightarrow{\mathbf{R}} \in \mathscr{L}} g(\overrightarrow{\mathbf{R}}) e^{-i\overrightarrow{\mathbf{k}}\cdot\overrightarrow{\mathbf{R}}}, \quad \overrightarrow{\mathbf{k}} \in FBZ$$

A.2. Proof of the Rotation Invariance of H_{Heis}

The commutator between the Heisenberg Hamiltonian and rotation operator can be written as:

$$\begin{aligned}[H_{Heis}, U(\alpha, u)] &= -J \sum_{<i,j>} [\exp\{i\alpha\hat{u} \cdot \overrightarrow{S}_T\}, S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z] \\ &= -i\alpha J \exp\{i\alpha\hat{u} \cdot \overrightarrow{S}_T\} \sum_k \sum_{<i,j>} [u_x S_k^x + u_y S_k^y + u_z S_k^z, S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z] \quad \text{(A.4)}\end{aligned}$$

To calculate the remaining commutator in (A.1), let us take only the case S_k^x, since the other three components yield analogous results. We have then, for fixed k:

$$\begin{aligned}\sum_{<i,j>} [S_k^x, S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z] &= [S_i^x, S_i^y] S_j^y + [S_i^x, S_i^z] S_j^z + S_i^y [S_j^x, S_j^y] + S_i^z [S_j^x, S_j^z] \\ &= i S_i^z S_j^y - i S_i^y S_j^z + i S_i^y S_j^z - i S_i^z S_j^y = 0 \quad \text{(A.5)}\end{aligned}$$

Analogously, one has:

$$\sum_{<i,j>} [S_k^y, S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z] = 0 \tag{A.6}$$

$$\sum_{<i,j>} [S_k^z, S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z] = 0 \tag{A.7}$$

Therefore, each k-term in the full commutator is null, which proves that:

$$[H_{Heis}, U(\alpha, u)] = 0 \tag{A.8}$$

Q.E.D.

A.3. Proof of the Holstein-Primakoff Representation

To prove that the representation (1.15) preserves the algebra of the spin operators, we just need to calculate the commutators $\left[S_i^{\pm}, S_i^z\right]$ and $\left[S_i^+, S_i^-\right]$ directly, and check if the results coincide with (1.6).

$$\begin{aligned}
\left[S_i^+, S_i^-\right] &= [\sqrt{2s - a_i^\dagger a_i} a_i, a_i^\dagger \sqrt{2s - a_i^\dagger a_i}] = \\
&= \sqrt{2s - a_i^\dagger a_i} a_i a_i^\dagger \sqrt{2s - a_i^\dagger a_i} - a_i^\dagger \left(2s - a_i^\dagger a_i\right) a_i = \\
&= \sqrt{2s - a_i^\dagger a_i} \left(a_i^\dagger a_i + \left[a_i, a_i^\dagger\right]\right) \sqrt{2s - a_i^\dagger a_i} - a_i^\dagger \left(2s - a_i a_i^\dagger + \left[a_i, a_i^\dagger\right]\right) a_i = \\
&= \left(2s - a_i^\dagger a_i\right) \left(a_i^\dagger a_i + 1\right) - a_i^\dagger a_i \left(2s - a_i^\dagger a_i\right) - a_i^\dagger a_i = \\
&= 2s - 2a_i^\dagger a_i = 2S_i^z
\end{aligned}$$

$$\begin{aligned}
\left[S_i^+, S_i^z\right] &= [\sqrt{2s - a_i^\dagger a_i} a_i, s - a_i^\dagger a_i] = -\sqrt{2s - a_i^\dagger a_i} \left[a_i, a_i^\dagger a_i\right] \\
&= -\sqrt{2s - a_i^\dagger a_i} a_i = -S_i^+
\end{aligned}$$

$$\begin{aligned}
\left[S_i^-, S_i^z\right] &= [a_i^\dagger \sqrt{2s - a_i^\dagger a_i}, s - a_i^\dagger a_i] = -\sqrt{2s - a_i^\dagger a_i} \left[a_i^\dagger, a_i^\dagger a_i\right] \\
&= a_i^\dagger \sqrt{2s - a_i^\dagger a_i} a_i = S_i^-
\end{aligned}$$

Q.E.D.

A.4. Rotation of Spin Operators

In general, one knows that the following formula is true for any non-commuting operators X and Y:

$$e^X Y e^{-X} = Y + \sum_{k=1}^{+\infty} \frac{[X,Y]_k}{k!}; \quad where\ [X,Y]_k = [X,[X\,[\ .....(k\ times)....Y]] \tag{A.9}$$

Furthermore, the rotation of a local operator $\mathcal{O}_i$ by an angle θ around the y-axis is implemented by $\widetilde{\mathcal{O}}_i = U(\theta)\mathcal{O}_i U(\theta)^\dagger$, where $U(\theta) = e^{i\theta S_i^y}$is the unitary rotation operator (of site i), defined as usual. Using the formula (A.6), we can write:

$$\begin{aligned} e^{i\theta S_i^y} S_i^z e^{-i\theta S_i^y} &= S_i^z + i\theta\,[S_i^y, S_i^z] - \frac{\theta^2}{2}\,[S_i^y,[S_i^y,S_i^z]] - i\frac{\theta^3}{6}\,[S_i^y,[S_i^y,[S_i^y,S_i^z]]] + ... \\ &= S_i^z - \theta S_i^x - \frac{\theta^2}{2} S_i^z + \frac{\theta^3}{6} S_i^x + ... = S_i^z(1 - \frac{\theta^2}{2!} + ...) - S_i^x(\theta - \frac{\theta^3}{3!} + ...) \\ &= S_i^z \cos\theta - S_i^x \sin\theta \end{aligned} \tag{A.10}$$

$$\begin{aligned} e^{i\theta S_i^y} S_i^x e^{-i\theta S_i^y} &= S_i^x + i\theta\,[S_i^y, S_i^x] - \frac{\theta^2}{2}\,[S_i^y,[S_i^y,S_i^x]] - i\frac{\theta^3}{6}\,[S_i^y,[S_i^y,[S_i^y,S_i^x]]] + ... \\ &= S_i^x + \theta S_i^z - \frac{\theta^2}{2} S_i^x - \frac{\theta^3}{6} S_i^z + ... = S_i^x(1 - \frac{\theta^2}{2!} + ...) + S_i^z(\theta - \frac{\theta^3}{3!} + ...) \\ &= S_i^x \cos\theta + S_i^z \sin\theta \end{aligned} \tag{A.11}$$

$$e^{i\theta S_i^y} S_i^y e^{-i\theta S_i^y} = S_i^y \tag{A.12}$$

In the same way, we can write the rotated ladder operators as follows:

$$e^{i\theta S_i^y} S_i^\pm e^{-i\theta S_i^y} = e^{i\theta S_i^y}\,(S_i^x \pm i S_i^y)\,e^{-i\theta S_i^y} = S_i^x \cos\theta + S_i^z \sin\theta \pm i S_i^y \tag{A.13}$$

Finally, by replacing $\theta = \pi$, we get the results (1.36).

It is also useful to write down the rotated spin operators, when the rotation is performed about the z-axis. Applying the same procedure, we get:

$$e^{i\theta S_i^z} S_i^x e^{-i\theta S_i^z} = S_i^x \cos\theta - S_i^y \sin\theta \tag{A.14}$$

$$e^{i\theta S_i^z} S_i^y e^{-i\theta S_i^z} = S_i^y \cos\theta + S_i^x \sin\theta \tag{A.15}$$

$$e^{i\theta S_i^z} S_i^z e^{-i\theta S_i^z} = S_i^z \tag{A.16}$$

In conclusion, the spin ladder-operators transform as if they were the $m = \pm 1$ elements of a spin-1 representation of $SO(3)$, yielding:

$$e^{i\theta S_i^z} S_i^{\pm} e^{-i\theta S_i^z} = e^{i\theta S_i^z} \left(S_i^x \pm i S_i^y\right) e^{-i\theta S_i^z} = e^{\pm i\theta} S_i^{\pm} \tag{A.17}$$

A.5. Diagonalization of the AFM Holstein-Primakoff Hamiltonian

In this appendix, the full diagonalization of the AFM Spin-Wave Hamiltonian is carried on. For a start, we remind the expression of the Hamiltonian in the original single-particle basis:

$$H_{SW} = H_{Heis} + Js^2 Nz = -JNzs \sum_{\mathbf{k}\in FBZ_{sub}} \left\{ \frac{\gamma_{\mathbf{k}}}{z} \left[a_{\mathbf{k}} b_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger\right] - \left[b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right]\right\} \tag{A.18}$$

And the tranformation to the new basis is given by:

$$\begin{cases} a_{\mathbf{k}} = u_{\mathbf{k}}^* c_{\mathbf{k}} + v_{\mathbf{k}} d_{-\mathbf{k}}^\dagger \\ a_{\mathbf{k}}^\dagger = u_{\mathbf{k}} c_{\mathbf{k}}^\dagger + v_{\mathbf{k}}^* d_{-\mathbf{k}} \end{cases} \qquad \begin{cases} b_{\mathbf{k}} = u_{\mathbf{k}}^* d_{\mathbf{k}} + v_{\mathbf{k}} c_{-\mathbf{k}}^\dagger \\ b_{\mathbf{k}}^\dagger = u_{\mathbf{k}} d_{\mathbf{k}}^\dagger + v_{\mathbf{k}}^* c_{-\mathbf{k}} \end{cases}$$

Replacing the expressions for the $c_{\mathbf{k}}$'s and $d_{\mathbf{k}}$'s in each of the quadratic terms inside the sum, we get:

$$\begin{aligned}
a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger &= \left(u_{\mathbf{k}} c_{\mathbf{k}}^\dagger + v_{\mathbf{k}}^* d_{-\mathbf{k}}\right)\left(u_{\mathbf{k}} d_{-\mathbf{k}}^\dagger + v_{\mathbf{k}}^* c_{\mathbf{k}}\right) = u_{\mathbf{k}}^2 c_{\mathbf{k}}^\dagger d_{-\mathbf{k}}^\dagger + v_{\mathbf{k}}^* u_{\mathbf{k}} d_{-\mathbf{k}}^\dagger d_{-\mathbf{k}} + u_{\mathbf{k}} v_{\mathbf{k}}^* c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + v_{\mathbf{k}}^{*2} d_{-\mathbf{k}} c_{\mathbf{k}} + v_{\mathbf{k}}^* u_{\mathbf{k}} \\
a_{\mathbf{k}} b_{-\mathbf{k}} &= \left(u_{\mathbf{k}}^* c_{\mathbf{k}} + v_{\mathbf{k}} d_{-\mathbf{k}}^\dagger\right)\left(u_{\mathbf{k}}^* d_{-\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}}^\dagger\right) = u_{\mathbf{k}}^{*2} c_{\mathbf{k}} d_{-\mathbf{k}} + v_{\mathbf{k}} u_{\mathbf{k}}^* d_{-\mathbf{k}}^\dagger d_{-\mathbf{k}} + u_{\mathbf{k}}^* v_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + v_{\mathbf{k}}^2 d_{-\mathbf{k}}^\dagger c_{\mathbf{k}}^\dagger + v_{\mathbf{k}} u_{\mathbf{k}}^* \\
a_{\mathbf{k}}^\dagger a_{\mathbf{k}} &= \left(u_{\mathbf{k}} c_{\mathbf{k}}^\dagger + v_{\mathbf{k}}^* d_{-\mathbf{k}}\right)\left(u_{\mathbf{k}}^* c_{\mathbf{k}} + v_{\mathbf{k}} d_{-\mathbf{k}}^\dagger\right) = |u_{\mathbf{k}}|^2 c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + u_{\mathbf{k}} v_{\mathbf{k}} c_{\mathbf{k}}^\dagger d_{-\mathbf{k}}^\dagger + u_{\mathbf{k}}^* v_{\mathbf{k}}^* c_{\mathbf{k}} d_{-\mathbf{k}} + \\
&\quad + |v_{\mathbf{k}}|^2 d_{-\mathbf{k}}^\dagger d_{-\mathbf{k}} + |v_{\mathbf{k}}|^2 \\
b_{\mathbf{k}}^\dagger b_{\mathbf{k}} &= \left(u_{\mathbf{k}}^* d_{\mathbf{k}}^\dagger + v_{\mathbf{k}} c_{-\mathbf{k}}\right)\left(u_{\mathbf{k}} d_{\mathbf{k}} + v_{\mathbf{k}}^* c_{-\mathbf{k}}^\dagger\right) = |u_{\mathbf{k}}|^2 d_{\mathbf{k}}^\dagger d_{\mathbf{k}} + u_{\mathbf{k}}^* v_{\mathbf{k}}^* d_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger + u_{\mathbf{k}} v_{\mathbf{k}} c_{-\mathbf{k}} d_{\mathbf{k}} + \\
&\quad + |v_{\mathbf{k}}|^2 c_{-\mathbf{k}}^\dagger c_{-\mathbf{k}} + |v_{\mathbf{k}}|^2
\end{aligned}$$

And, by replacing these expressions into (A.15), we arrive at:

$$\begin{aligned}
&\sum_{\mathbf{k}\in FBZ_{sub}} \left\{\widetilde{\gamma}_{\mathbf{k}} \left[a_{\mathbf{k}} b_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger\right] - \left[b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right]\right\} = \\
&= \sum_{\mathbf{k}\in FBZ_{sub}} \left[c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \left\{\widetilde{\gamma}_{\mathbf{k}} \left[u_{\mathbf{k}} v_{\mathbf{k}}^* + u_{\mathbf{k}}^* v_{\mathbf{k}}\right] - |u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2\right\} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}} \left\{\widetilde{\gamma}_{\mathbf{k}} \left[u_{\mathbf{k}} v_{\mathbf{k}}^* + u_{\mathbf{k}}^* v_{\mathbf{k}}\right] - |u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2\right\}\right] + \\
&+ \sum_{\mathbf{k}\in FBZ_{sub}} \left[c_{\mathbf{k}}^\dagger d_{-\mathbf{k}}^\dagger \left\{\widetilde{\gamma}_{\mathbf{k}} \left[u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2\right] - u_{\mathbf{k}} v_{\mathbf{k}} - u_{\mathbf{k}}^* v_{\mathbf{k}}^*\right\} + d_{-\mathbf{k}} c_{\mathbf{k}} \left\{\widetilde{\gamma}_{\mathbf{k}} \left[u_{\mathbf{k}}^{*2} + v_{\mathbf{k}}^{*2}\right] - u_{\mathbf{k}}^* v_{\mathbf{k}}^* - u_{\mathbf{k}} v_{\mathbf{k}}\right\}\right] - \\
&+ \sum_{\mathbf{k}\in FBZ_{sub}} \left[\widetilde{\gamma}_{\mathbf{k}} \left\{v_{\mathbf{k}}^* u_{\mathbf{k}} + v_{\mathbf{k}} u_{\mathbf{k}}^*\right\} - 2|v_{\mathbf{k}}|^2\right]
\end{aligned} \tag{A.19}$$

We can assume that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are real numbers, as long as they keep respecting the constraint $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$, therefore we get:

$$\sum_{\mathbf{k}\in FBZ_{sub}}\left[\widetilde{\gamma}_{\mathbf{k}}\left[a_{\mathbf{k}}b_{-\mathbf{k}}+a_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger}\right]-b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}-a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right]=$$
$$=-\sum_{\mathbf{k}\in FBZ_{sub}}\left[\left\{c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}+d_{\mathbf{k}}^{\dagger}d_{\mathbf{k}}\right\}\left\{u_{\mathbf{k}}^{2}+v_{\mathbf{k}}^{2}-2\widetilde{\gamma}_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}\right\}+\left\{c_{\mathbf{k}}^{\dagger}d_{-\mathbf{k}}^{\dagger}+d_{-\mathbf{k}}c_{\mathbf{k}}\right\}\left\{2u_{\mathbf{k}}v_{\mathbf{k}}-\widetilde{\gamma}_{\mathbf{k}}\left[u_{\mathbf{k}}^{2}+v_{\mathbf{k}}^{2}\right]\right\}\right]+$$
$$+\sum_{\mathbf{k}\in FBZ_{sub}}\left[2\widetilde{\gamma}_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}}-2v_{\mathbf{k}}^{2}\right]$$

Where $\widetilde{\gamma}_{\mathbf{k}}=\frac{\gamma_{\mathbf{k}}}{z}$. Now, we want the anomalous terms to disappear, leaving only the diagonal part of the above expression. To do that, we must impose that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, besides obeying (1.45), are also solutions of $\gamma_{\mathbf{k}}\left[u_{\mathbf{k}}^{2}+v_{\mathbf{k}}^{2}\right]-2u_{\mathbf{k}}v_{\mathbf{k}}=0$, for all $\mathbf{k}\in FBZ$. Let's then calculate one solution of these:

$$\begin{cases}\widetilde{\gamma}_{\mathbf{k}}\left[u_{\mathbf{k}}^{2}+v_{\mathbf{k}}^{2}\right]=2u_{\mathbf{k}}v_{\mathbf{k}}\\ u_{\mathbf{k}}^{2}=1+v_{\mathbf{k}}^{2}\end{cases}\Rightarrow\begin{cases}\widetilde{\gamma}_{\mathbf{k}}\left[1+2v_{\mathbf{k}}^{2}\right]=2\sqrt{1+v_{\mathbf{k}}^{2}}v_{\mathbf{k}}\\ u_{\mathbf{k}}^{2}=1+v_{\mathbf{k}}^{2}\end{cases}\Rightarrow\begin{cases}\widetilde{\gamma}_{\mathbf{k}}^{2}\left[1+4v_{\mathbf{k}}^{2}+4v_{\mathbf{k}}^{4}\right]=4v_{\mathbf{k}}^{2}+4v_{\mathbf{k}}^{4}\\ u_{\mathbf{k}}^{2}=1+v_{\mathbf{k}}^{2}\end{cases}$$
$$\Rightarrow\begin{cases}\widetilde{\gamma}_{\mathbf{k}}^{2}\left[1+4v_{\mathbf{k}}^{2}+4v_{\mathbf{k}}^{4}\right]=4v_{\mathbf{k}}^{2}+4v_{\mathbf{k}}^{4}\\ u_{\mathbf{k}}^{2}=1+v_{\mathbf{k}}^{2}\end{cases}\Rightarrow\begin{cases}4(1-\widetilde{\gamma}_{\mathbf{k}}^{2})v_{\mathbf{k}}^{4}+4(1-\widetilde{\gamma}_{\mathbf{k}}^{2})v_{\mathbf{k}}^{2}-\widetilde{\gamma}_{\mathbf{k}}^{2}=0\\ u_{\mathbf{k}}^{2}=1+v_{\mathbf{k}}^{2}\end{cases}\tag{A.20}$$

To solve the top equation, we can change variables — $x\equiv 2\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}v_{\mathbf{k}}^{2}$ — which gets us to the following quadratic equation:

$$x^{2}+2\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}x-\gamma_{\mathbf{k}}^{2}=0\Rightarrow x=-\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}\pm 1\tag{A.21}$$

Choosing the positive roots, we can write:

$$v_{\mathbf{k}}=\sqrt{\frac{1}{2\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}}-\frac{1}{2}}\tag{A.22}$$

$$u_{\mathbf{k}}=\sqrt{\frac{1}{2\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}}+\frac{1}{2}}\tag{A.23}$$

From which, we see that — $u_{\mathbf{k}}^{2}+v_{\mathbf{k}}^{2}-2\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}=\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}$ — and — $2\widetilde{\gamma}_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}}-2v_{\mathbf{k}}^{2}=-\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}+1$ — and end up with the following diagonal Hamiltonian:

$$H_{SW}=2Jzs\sum_{\mathbf{k}\in FBZ_{sub}}\left[\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}\left\{c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}+d_{\mathbf{k}}^{\dagger}d_{\mathbf{k}}\right\}\right]+2Jzs\sum_{\mathbf{k}\in FBZ_{sub}}\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}-JzNs\tag{A.24}$$

$$=Jzs\sum_{\mathbf{k}\in FBZ_{sub}}\left[\sqrt{1-\widetilde{\gamma}_{\mathbf{k}}^{2}}\left\{c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}+d_{\mathbf{k}}^{\dagger}d_{\mathbf{k}}+1\right\}\right]-JzNs\tag{A.25}$$

B. Appendix

B.1. The Bogoliubov Inequality

In this Appendix, we will prove the Bogoliubov inequality used in Section 2.2. This is essentially a basic result on operators acting in an arbitrary Hilbert space $\mathscr{H}$ spanned by a set of eigenvectors of an arbitrary Hamiltonian H. Let us call the basis vectors $\{|\phi_i\rangle\}_i$, where i labels the state, and can be either a discrete or continuous variable. Furthermore, we have $H|\phi_i\rangle = E_i|\phi_i\rangle$.

Now, given two arbitrary bounded linear operators[1] acting on $\mathscr{H}$, called A,$B \in End(\mathscr{H})$, we define a non-definite internal product in the linear space of operators $End(\mathscr{H})$, as follows:

$$(A,B) \equiv \frac{1}{Z(T)} \sum_i \sum_{j(E_j \neq E_i)} \langle\phi_j| A^\dagger |\phi_i\rangle \langle\phi_i| B |\phi_j\rangle \frac{e^{-\beta E_i} - e^{-\beta E_j}}{E_j - E_i}$$

It is obvious that it is linear and symmetrical (in the complex sense), i.e.:

$$(A,B) = (B,A)^*$$
$$(A, \mu B + \nu C) = \mu (A,B) + \nu (A,C)$$

It remains to be proven that it is also positive[2]. This is a simple proof though, since we know that $0 < \frac{e^{-\beta E_i} - e^{-\beta E_j}}{E_j - E_i}$, meaning that:

$$(A,A) = \frac{1}{Z(T)} \sum_i \sum_{j(E_j \neq E_i)} \left|\langle\phi_j| A^\dagger |\phi_i\rangle\right|^2 \frac{e^{-\beta E_i} - e^{-\beta E_j}}{E_j - E_i} \geq 0$$

Finally, any positive internal product obeys the Cauchy-Schwartz Inequality, which means that:

$$(A,A)(B,B) \geq |(A,B)|^2$$

Now, using the last inequality, we can reach the intended result, as follows. First, we must choose $B = \left[C^\dagger, H\right]$, where C is any given operator and H is the Hamiltonian. This directly yields:

[1] An operator is bounded if all of its matrix elements with respect to a given basis are finite.
[2] Although clearly not positive definite, since, for example $(\mathbb{I}, \mathbb{I}) = 0$.

$$(A,B) = \left(A, \left[C^\dagger, H\right]\right) = \frac{1}{Z(T)} \sum_i \sum_{j(E_j \neq E_i)} \langle \phi_j | A^\dagger | \phi_i \rangle \langle \phi_i | C^\dagger H - H C^\dagger | \phi_j \rangle \frac{e^{-\beta E_i} - e^{-\beta E_j}}{E_j - E_i} =$$
$$= \frac{1}{Z(T)} \sum_i \sum_{j(E_j \neq E_i)} \langle \phi_j | A^\dagger | \phi_i \rangle \langle \phi_i | C^\dagger E_j - E_i C^\dagger | \phi_j \rangle \frac{e^{-\beta E_i} - e^{-\beta E_j}}{E_j - E_i} =$$
$$= \frac{1}{Z(T)} \sum_i \sum_{j(E_j \neq E_i)} \left[\langle \phi_i | C^\dagger | \phi_j \rangle \langle \phi_j | A^\dagger | \phi_i \rangle e^{-\beta E_i} - \langle \phi_j | A^\dagger | \phi_i \rangle \langle \phi_i | C^\dagger | \phi_j \rangle e^{-\beta E_j} \right] =$$
$$= \frac{1}{Z(T)} \left[\sum_i \langle \phi_i | C^\dagger A^\dagger | \phi_i \rangle e^{-\beta E_i} - \sum_j \langle \phi_j | A^\dagger C^\dagger | \phi_j \rangle e^{-\beta E_j} \right] = \left\langle \left[C^\dagger, A^\dagger\right] \right\rangle_T$$

This equation immediately implies that:

$$(B,B) = \left\langle \left[C^\dagger, \left[C^\dagger, H\right]^\dagger\right] \right\rangle_T = \left\langle \left[C^\dagger, [H,C]\right] \right\rangle_T$$

On the other hand, we can also bound the norm of the operator A, by the average of the anticommutator with its hermitian conjugate. This can be done if we notice the following trivial inequality ($\tanh x \leq x$):

$$0 \leq \frac{e^{-\beta E_i} - e^{-\beta E_j}}{E_j - E_i} = \frac{e^{-\beta E_i} + e^{-\beta E_j}}{E_j - E_i} \tanh\left[\frac{\beta}{2}(E_j - E_i)\right] \leq \frac{\beta}{2}\left(e^{-\beta E_i} + e^{-\beta E_j}\right)$$

Using the above inequality in the expression for the norm of A, we get:

$$0 \leq (A,A) \leq \frac{\beta}{2Z(T)} \sum_i \sum_{j(E_j \neq E_i)} \langle \phi_j | A^\dagger | \phi_i \rangle \langle \phi_i | A | \phi_j \rangle \left(e^{-\beta E_i} + e^{-\beta E_j}\right) =$$
$$= \frac{\beta}{2Z(T)} \left[\sum_i \langle \phi_i | A A^\dagger | \phi_i \rangle e^{-\beta E_i} + \sum_j \langle \phi_j | A^\dagger A | \phi_j \rangle e^{-\beta E_j} \right] = \frac{\beta}{2} \left\langle \left\{A, A^\dagger\right\} \right\rangle_T$$

At last, we can plug in the previous 3 results into the original Cauchy-Schwartz Inequality, arriving at the general expression of the famous Bogoliubov inequality:

$$\left\langle \left\{A, A^\dagger\right\} \right\rangle_T \left\langle \left[C^\dagger, [H,C]\right] \right\rangle_T \geq 2k_B T \left| \left\langle \left[C^\dagger, A^\dagger\right] \right\rangle_T \right|^2 \tag{B.1}$$

B.2. Exact Solution of the Infinite Range AFM Model

In this Appendix, we carry on with the diagonalization of the manybody Hamiltonian (2.50), which reads:

$$H_{IRQAFM} = J \sum_{i \in \mathscr{L}_A} \sum_{j \in \mathscr{L}_B} \overrightarrow{S}_i \cdot \overrightarrow{S}_j = J \overrightarrow{S}_{TotA} \cdot \overrightarrow{S}_{TotB} \quad with\ J > 0$$

To turn the above Hamiltonian in a clearly manageable form, one can just notice that $\overrightarrow{S}_{Tot} = \overrightarrow{S}_{TotA} + \overrightarrow{S}_{TotB}$, which means that:

$$S^2_{Tot} = S^2_{TotA} + S^2_{TotB} + 2\overrightarrow{S}_{TotA} \cdot \overrightarrow{S}_{TotB} \Rightarrow \overrightarrow{S}_{TotA} \cdot \overrightarrow{S}_{TotB} = \frac{1}{2}\left[S^2_{Tot} - S^2_{TotA} - S^2_{TotB}\right]$$

Which yields the trivial Hamiltonian:

$$H_{IRQAFM} = \frac{J}{2}\left[S^2_{Tot} - S^2_{TotA} - S^2_{TotB}\right]$$

Now, since we know that $\left[S^2_{TotA}, S^2_{TotB}\right] = \left[S^2_{Tot}, S^2_{TotB}\right] = \left[S^2_{Tot}, S^2_{TotA}\right] = 0$, we can take the common eigenstates of these operators - $|S_{tot}, S_{TotA}, S_{TotB}, \mu\rangle$ - (where μ are further quantum numbers necessary to catalog all the states with the same energy) relative to which we get:

$$\begin{aligned} H_{IRQAFM}\,|S_{tot}, S_{TotA}, S_{TotB}, \mu\rangle = \frac{J}{2}\left[S_{tot}\left(S_{tot}+1\right) - S_{totA}\left(S_{totA}+1\right) - \right. \\ \left. - S_{totA}\left(S_{totA}+1\right)\right]|S_{tot}, S_{TotA}, S_{TotB}, \mu\rangle \end{aligned}$$

Therefore the spectrum of the model is:

$$E_\infty(S_{tot}, S_{TotA}, S_{TotB}) = \frac{J}{2}\left[S_{tot}\left(S_{tot}+1\right) - S_{totA}\left(S_{totA}+1\right) - S_{totA}\left(S_{totA}+1\right)\right]$$

As mentioned in the main text.

As a final comment, we may notice also that $\left[S^2_{Tot}, S^z_{Tot}\right] = \left[S^2_{TotA}, S^z_{Tot}\right] = \left[S^2_{TotB}, S^z_{Tot}\right] = 0$, which makes M a good quantum number that can completely catalog a complete basis of the total Hilbert Space. Therefore, the eigenstates of H_{IRQAFM} can be chosen to be the states $|S_{tot}, M; S_{TotA}, S_{TotB}\rangle$.

B.3. Derivation of the Twisted Heisenberg Hamiltonian

In this appendix, we do the detailed derivation of the Heisenberg Hamiltonian after the twisting transformation induced by the operator $\mathcal{O}^1$:

$$\begin{aligned} \mathcal{O}^{1\dagger} H_{Heis} \mathcal{O}^1 = \prod_{j=1}^{N} \exp\left(-i\frac{2\pi}{N} j S^z_j\right) \left\{ J \sum_{j=1}^{N-1} \left[1/2 \left\{ S^+_j S^-_{j+1} + S^-_j S^+_{j+1} \right\} + S^z_j S^z_{j+1} \right] + \right. \\ \left. + J\left[1/2 \left\{ S^+_N S^-_1 + S^-_N S^+_1 \right\} + S^z_N S^z_1 \right] \right\} \prod_{j=1}^{N} \exp\left(i\frac{2\pi}{N} j S^z_j\right) \end{aligned}$$

To do the above calculation, it is enough to obtain the transformation law for each pair-interaction term, such as:

$$
\begin{aligned}
&\mathcal{O}^{1\dagger}\left[1/2\left\{S_j^+S_i^- + S_j^-S_i^+\right\} + S_j^zS_i^z\right]\mathcal{O}^1 = \\
&= 1/2\exp\left(-i\frac{2\pi}{N}jS_j^z\right)S_j^+\exp\left(-i\frac{2\pi}{N}jS_j^z\right)\exp\left(-i\frac{2\pi}{N}jS_i^z\right)S_i^-\exp\left(-i\frac{2\pi}{N}jS_i^z\right) + \\
&+ 1/2\exp\left(-i\frac{2\pi}{N}jS_j^z\right)S_j^-\exp\left(-i\frac{2\pi}{N}jS_j^z\right)\exp\left(-i\frac{2\pi}{N}jS_i^z\right)S_i^+\exp\left(-i\frac{2\pi}{N}jS_i^z\right) + S_j^zS_i^z \\
&= 1/2\left\{e^{i\frac{2\pi}{N}(j-i)}S_j^+S_i^- + e^{-i\frac{2\pi}{N}(j-i)}S_j^-S_i^+\right\} + S_j^zS_i^z \quad \text{[using Appendix A.4]}
\end{aligned}
$$

Applying this last result to the original expression of the Hamiltonian, we can obtain the desired result:

$$
\begin{aligned}
\mathcal{O}^{1\dagger}H_{Heis}\mathcal{O}^1 = H_{Heis} + \frac{J}{2}\sum_{j=1}^{N-1}\left[\left(e^{i\frac{2\pi}{N}}-1\right)S_j^+S_{j+1}^- + \left(e^{-i\frac{2\pi}{N}}-1\right)S_j^-S_{j+1}^+\right] + \\
+ \frac{J}{2}\left[\left(e^{-i\frac{2\pi}{N}}-1\right)S_N^+S_1^- + \left(e^{i\frac{2\pi}{N}}-1\right)S_N^-S_1^+\right]
\end{aligned}
$$

Taking the average of this expression with respect to the state $|\Psi_0\rangle$ will produce the expression (2.54).

C. Appendix

C.1. Properties of the Schwinger Bosons

In this Appendix we will derive some important results on the 2-boson representation of spin operators, that was first defined in Chapter 3. We start by proving that the definitions:

$$S^+ = a^\dagger b \quad S^- = b^\dagger a \quad S^z = 1/2 \left\{ a^\dagger a - b^\dagger b \right\}$$

$$\left[a, a^\dagger \right] = \left[b, b^\dagger \right] = 1 \quad [a, a] = [b, b] = [a, b] = \left[a, b^\dagger \right] = 0$$

Indeed produce the correct algebra for the operators $S^\pm$ and S^z (i.e. equations (1.6)). This is done directly as follows:

$$\left[S^+, S^- \right] = \left[a^\dagger b, b^\dagger a \right] = -b^\dagger \left[a, a^\dagger \right] b + a^\dagger \left[b, b^\dagger \right] a = a^\dagger a - b^\dagger b = 2S^z$$

$$\left[S^+, S^z \right] = 1/2 \left[a^\dagger b, a^\dagger a - b^\dagger b \right] = 1/2 \left\{ -a^\dagger \left[a, a^\dagger \right] b - a^\dagger \left[b, b^\dagger \right] b \right\} = -S^+$$

$$\left[S^-, S^z \right] = 1/2 \left[b^\dagger a, a^\dagger a - b^\dagger b \right] = 1/2 \left\{ b^\dagger \left[a, a^\dagger \right] a - b^\dagger \left[b, b^\dagger \right] a \right\} = S^-$$

Furthermore, the total spin operator $S^2 = 1/2 \{ S^+ S^- + S^- S^+ \} + S^z S^z$ can also be written in terms of Schwinger bosonic operators, i.e.:

$$S^2 = 1/2 \left\{ a^\dagger a b b^\dagger + a a^\dagger b^\dagger b \right\} + 1/4 \left\{ \left(a^\dagger a \right)^2 + \left(b^\dagger b \right)^2 + 2 a^\dagger a b^\dagger b \right\} = \left(\frac{a^\dagger a}{2} + \frac{b^\dagger b}{2} \right) \left(\left(\frac{a^\dagger a}{2} + \frac{b^\dagger b}{2} \right) + 1 \right)$$

What justifies the identification of the Fock state $|n_a, n_b\rangle$ with the standard spin state:

$$|s = 1/2 \left[n_a + n_b \right]; \quad m = 1/2 \left[n_a - n_b \right] \rangle$$

As was referred in the text.

Besides building the the spin operators, we also need to know how do the bosonic operators transform when acted by a space rotation. To do that, (following Ref. [19]) we start by calculating the commutation relations between the spin components and the Schwinger creation operators, i.e.:

$$\left[S^x, a^\dagger\right] = \left[1/2\left(S^- + S^+\right), a^\dagger\right] = \left[1/2\left(a^\dagger b + b^\dagger a\right), a^\dagger\right] = 1/2 b^\dagger$$

$$\left[S^x, b^\dagger\right] = \left[1/2\left(S^- + S^+\right), b^\dagger\right] = \left[1/2\left(a^\dagger b + b^\dagger a\right), a^\dagger\right] = 1/2 a^\dagger$$

$$\left[S^y, a^\dagger\right] = \left[-i/2\left(S^+ - S^-\right), a^\dagger\right] = -\left[i/2\left(a^\dagger b - b^\dagger a\right), a^\dagger\right] = i/2 b^\dagger$$

$$\left[S^y, b^\dagger\right] = \left[-i/2\left(S^- - S^+\right), b^\dagger\right] = -\left[i/2\left(a^\dagger b - b^\dagger a\right), a^\dagger\right] = -i/2 a^\dagger$$

$$\left[S^z, a^\dagger\right] = 1/2 a^\dagger, \quad \left[S^z, b^\dagger\right] = -1/2 b^\dagger$$

Now, a rotation of angle θ around any of this axis (in the positive sense) can be expressed by an unitary operator. As we will need only rotations around the $y-$ and $z-$axis, we will explicitly calculate the transformation law for $a^\dagger/b^\dagger$ only in these two cases. That goes as follows:

For the $y-$axis:

$$\begin{aligned} U_y(\theta) a^\dagger U_y(\theta)^\dagger &= e^{-i\theta S^y} a^\dagger e^{i\theta S^y} = a^\dagger + \sum_{k=1}^{\infty} \frac{\left[S^y, a^\dagger\right]_k}{k!} (-i\theta)^k = \\ &= a^\dagger \cos(\theta/2) + b^\dagger \sin(\theta/2) \end{aligned}$$

$$\begin{aligned} U_y(\theta) b^\dagger U_y(\theta)^\dagger &= e^{-i\theta S^y} b^\dagger e^{i\theta S^y} = b^\dagger + \sum_{k=1}^{\infty} \frac{\left[S^y, b^\dagger\right]_k}{k!} (-i\theta)^k = \\ &= b^\dagger \cos(\theta/2) - a^\dagger \sin(\theta/2) \end{aligned}$$

For the $z-$axis:

$$\begin{aligned} U_z(\phi) a^\dagger U_z(\phi)^\dagger &= e^{-i\phi S^z} a^\dagger e^{i\phi S^z} = a^\dagger + \sum_{k=1}^{\infty} \frac{\left[S^z, a^\dagger\right]_k}{k!} (-i\phi)^k = \\ &= e^{-i\phi/2} a^\dagger \end{aligned}$$

$$\begin{aligned} U_z(\phi) b^\dagger U_z(\phi)^\dagger &= e^{-i\phi S^z} b^\dagger e^{i\phi S^z} = b^\dagger + \sum_{k=1}^{\infty} \frac{\left[S^z, b^\dagger\right]_k}{k!} (-i\phi)^k = \\ &= e^{i\phi/2} b^\dagger \end{aligned}$$

Using this, we can readily obtain the needed result (3.9):

$$\widetilde{\begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix}} = U_z(\phi)U_y(\theta)\begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix}U_y(\theta)^\dagger U_z(\phi)^\dagger = \begin{pmatrix} e^{-i\phi/2}\cos(\theta/2)a^\dagger + e^{i\phi/2}\sin(\theta/2)b^\dagger \\ e^{i\phi/2}\cos(\theta/2)b^\dagger - e^{-i\phi/2}\sin(\theta/2)a^\dagger \end{pmatrix} =$$
$$= \begin{pmatrix} e^{-i\phi/2}\cos(\theta/2) & e^{i\phi/2}\sin(\theta/2) \\ -e^{-i\phi/2}\sin(\theta/2) & e^{i\phi/2}\cos(\theta/2) \end{pmatrix} \cdot \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix}$$

Finally, we state the transformation property for the creation Schwinger operators, under a rotation of Euler angles $(\phi, \theta, \chi = 0)$.

$$\begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix} \longmapsto \begin{pmatrix} e^{-i\phi/2}\cos(\theta/2) & e^{i\phi/2}\sin(\theta/2) \\ -e^{-i\phi/2}\sin(\theta/2) & e^{i\phi/2}\cos(\theta/2) \end{pmatrix} \cdot \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix}$$

C.2. Heisenberg Uncertainty Relation Among Spin Components

In this Appendix we will derive the uncertainty relation (3.5) from the non-abelian algebra os the spin components. To do that, we start by noticing that the average of two hermitian operators obeys the following inequality:

$$|\langle AB\rangle| \leq \langle A^2\rangle \langle B^2\rangle$$

This is proven just by taking two states $|\phi_1\rangle = A|\Psi\rangle$ and $|\phi_2\rangle = B|\Psi\rangle$. The inner product among these two states verifies the Cauchy-Schwarz inequality, i.e.:

$$|\langle \phi_1 \mid \phi_2\rangle| \leq \sqrt{\langle \phi_1 \mid \phi_1\rangle}\sqrt{\langle \phi_2 \mid \phi_2\rangle}$$

Or, using the definition of these states:

$$|\langle\Psi| AB |\Psi\rangle| \leq \sqrt{\langle\Psi| A^2 |\Psi\rangle}\sqrt{\langle\Psi| B^2 |\Psi\rangle}$$

We get the desired formula.

Now, we set $A = \Delta S^x = S^x - \langle S^x\rangle$ and $B = \Delta S^y = S^y - \langle S^y\rangle$. Hence, we get:

$$\sqrt{\left\langle (\Delta S^x)^2 \right\rangle \left\langle (\Delta S^y)^2 \right\rangle} \geq |\langle \Delta S^x \Delta S^y\rangle| = |\langle S^x S^y - S^x \langle S^y\rangle - S^y \langle S^x\rangle + \langle S^x\rangle \langle S^y\rangle\rangle|$$

Since the states we are averaging over are symmetric with respect to rotations around the z-axis [i.e. they are $|s,m\rangle$ states.], we know that $\langle \Delta S^x \Delta S^y \rangle = \langle \Delta S^y \Delta S^x \rangle$. Applying this result to the last inequality we can write it as follows:

$$\begin{aligned}\sqrt{\left\langle (\Delta S^x)^2 \right\rangle \left\langle (\Delta S^y)^2 \right\rangle} \geq {}& 1/2 \left| \langle S^x S^y - S^x \langle S^y \rangle - S^y \langle S^x \rangle + \langle S^x \rangle \langle S^y \rangle \rangle \right| + \\ & + 1/2 \left| \langle S^y S^x - S^x \langle S^y \rangle - S^y \langle S^x \rangle + \langle S^x \rangle \langle S^y \rangle \rangle \right| \geq \\ & \geq 1/2 \left| \langle S^x S^y - S^y S^x \rangle \right| = 1/2 \left| \langle S^z \rangle \right|\end{aligned}$$

Where in the last inequality, use was made of the triangle inequality - $|a-b| \leq |a|+|b|$. Finally we can write the uncertainty relation for the components of the spin that are orthogonal to the quantization axis, as:

$$1/2 \left| \langle S^z \rangle \right| \leq \sqrt{\left\langle (\Delta S^x)^2 \right\rangle \left\langle (\Delta S^y)^2 \right\rangle}$$

Q.E.D.

C.3. Orthogonality and Completeness Relations of the Spin Coherent States

In this Appendix, we will derive the orthogonality and completeness relations for spin coherent states, obtaining the results — (3.12) and (3.13). We begin with the overlap function (3.12), where we took the definition (3.11) in terms of $|s,m\rangle$ states:

$$\begin{aligned}\langle \Omega_1^s \mid \Omega_2^s \rangle &= (2s)! \sum_{m_1=-s}^{s} \sum_{m_2=-s}^{s} \frac{(u_1^*)^{s+m_1} (v_1^*)^{s-m_1}}{\sqrt{(s+m_1)!\,(s-m_1)!}} \frac{u_2^{s+m_2} v_2^{s-m_2}}{\sqrt{(s+m_2)!\,(s-m_2)!}} \langle s, m_1 \mid s, m_2 \rangle = \\ &= (2s)! \sum_{m_1=-s}^{s} \sum_{m_2=-s}^{s} \frac{(u_1^*)^{s+m_1} (v_1^*)^{s-m_1}}{\sqrt{(s+m_1)!\,(s-m_1)!}} \frac{u_2^{s+m_2} v_2^{s-m_2}}{\sqrt{(s+m_2)!\,(s-m_2)!}} \delta_{m_1 m_2} = \\ &= \sum_{m=-s}^{s} \frac{(2s)!}{(s+m)!\,(s-m)!} (u_1^* u_2)^{s+m} (v_1^* \nu_2)^{s-m} = \\ &= \sum_{k=0}^{2s} \frac{(2s)!}{(k)!\,(2s-k)!} (u_1^* u_2)^{k} (v_1^* \nu_2)^{2s-k} = [u_1^* u_2 + v_1^* \nu_2]^{2s}\end{aligned} \tag{C.1}$$

Applying the definitions $u(\theta,\phi) = e^{-i\phi/2} \cos\theta/2$ and $v(\theta,\phi) = e^{i\phi/2} \sin\theta/2$ to the last result, we obtain:

$$\langle \Omega_1^s \mid \Omega_2^s \rangle = \left[\left(\cos\theta_1/2 \cos\theta_2/2 \cos\frac{\phi_2-\phi_1}{2} + \sin\theta_1/2 \sin\theta_2/2 \cos\frac{\phi_2-\phi_1}{2} \right) + \right.$$
$$\left. - i \left(\cos\theta_1/2 \cos\theta_2/2 \sin\frac{\phi_2-\phi_1}{2} - \sin\theta_1/2 \sin\theta_2/2 \sin\frac{\phi_2-\phi_1}{2} \right) \right]^{2s} \tag{C.2}$$

It is worth writing the above complex expression in the polar form — $\langle \Omega_1^s \mid \Omega_2^s \rangle = \rho e^{i\xi}$ — where:

$$\tan \xi/2s = -\frac{\cos\theta_1/2 \cos\theta_2/2 \sin\frac{\phi_2-\phi_1}{2} - \sin\theta_1/2 \sin\theta_2/2 \sin\frac{\phi_2-\phi_1}{2}}{\cos\theta_1/2 \cos\theta_2/2 \cos\frac{\phi_2-\phi_1}{2} + \sin\theta_1/2 \sin\theta_2/2 \cos\frac{\phi_2-\phi_1}{2}} =$$
$$= \tan\left(\frac{\phi_1-\phi_2}{2}\right) \frac{\cos\left(\frac{\theta_1+\theta_2}{2}\right)}{\cos\left(\frac{\theta_1-\theta_2}{2}\right)}$$

And also:

$$\rho^{1/s} = \cos^2\left(\frac{\theta_2-\theta_1}{2}\right)\cos^2\left(\frac{\phi_2-\phi_1}{2}\right) + \cos^2\left(\frac{\theta_2+\theta_1}{2}\right)\sin^2\left(\frac{\phi_2-\phi_1}{2}\right) =$$
$$= 1/4\left[1+\cos(\theta_2-\theta_1)\right]\left[1+\cos(\phi_2-\phi_1)\right] + 1/4\left[1+\cos(\theta_2+\theta_1)\right]\left[1-\cos(\phi_2-\phi_1)\right] =$$
$$= 1/2 + 1/4\left[\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\right]\left[1+\cos(\phi_2-\phi_1)\right] +$$
$$+ 1/4\left[\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2\right]\left[1-\cos(\phi_2-\phi_1)\right] =$$
$$= 1/2\left[1+\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_2-\phi_1)\right]$$

This last result may be casted in a more enlightening form, by recognizing that:

$$\Omega_1 \cdot \Omega_2 = \sin\theta_1\sin\theta_2\left[\cos\phi_1\cos\phi_2 + \sin\phi_1\sin\phi_2\right] + \cos\theta_1\cos\theta_2 =$$
$$= \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2) + \cos\theta_1\cos\theta_2 \tag{C.3}$$

In which case, we can write — $\rho = \left[\frac{1+\Omega_1\cdot\Omega_2}{2}\right]^s$ — allowing us to obtain the result quoted in (3.12):

$$\langle \Omega_2^s \mid \Omega_1^s \rangle = \left[\frac{1+\Omega_1\cdot\Omega_2}{2}\right]^s \exp\left[2si \arctan\left\{\tan\left(\frac{\phi_2-\phi_1}{2}\right)\frac{\cos\left(\frac{\theta_1+\theta_2}{2}\right)}{\cos\left(\frac{\theta_1-\theta_2}{2}\right)}\right\}\right]$$

Moving on to the derivation of the completeness relation (3.13), we start by writing the right-hand side in terms of $|s,m\rangle$ states, i.e.:

$$\left(\frac{2s+1}{4\pi}\right)\int_{S^2} d\Omega\,|\Omega^s\rangle\,\langle\Omega^s| =$$
$$= \left(\frac{2s+1}{4\pi}\right)\int_0^{2\pi} d\phi\int_0^{\pi}\sin\theta d\theta\left[(2s)!\sum_{m_1=-s}^{s}\sum_{m_2=-s}^{s}\frac{(u^*)^{s+m_1}\,(v^*)^{s-m_1}}{\sqrt{(s+m_1)!\,(s-m_1)!}}\times\right.$$
$$\left.\times\frac{u^{s+m_2}v^{s-m_2}}{\sqrt{(s+m_2)!\,(s-m_2)!}}\,|s,m_2\rangle\,\langle s,m_1|\right] \tag{C.4}$$

For each m_1 and m_2, we can write the integral (C.4) as follows:

$$\int_0^{2\pi} d\phi\int_0^{\pi}\cos\theta d\theta\,(u^*)^{s+m_1}\,(v^*)^{s-m_1}\,u^{s+m_2}v^{s-m_2} =$$
$$= \int_0^{2\pi} d\phi\int_0^{\pi}\cos\theta d\theta\,(\cos\theta/2)^{2s+m_1+m_2}\,(\sin\theta/2)^{2s-m_1-m_2}\,e^{i(m_2-m_1)\phi/2} \tag{C.5}$$

The integral over ϕ is clearly null when $m_1 \neq m_2$, and otherwise (C.5) can be written as:

$$\begin{aligned} I_{m,s} &= 4\pi\int_0^{\pi}\sin\theta d\theta\left(\frac{1+\cos\theta}{2}\right)^{s+m}\left(\frac{1-\cos\theta}{2}\right)^{s-m} = \\ &= -4\pi\int_1^{-1} du\left(\frac{1+u}{2}\right)^{s+m}\left(1-\frac{1+u}{2}\right)^{s-m} = \\ &= 4\pi\int_0^{1} dx x^{s+m}\,(1-x)^{s-m} \end{aligned} \tag{C.6}$$

Using the general result:

$$\int_0^1 dx x^m\,(1-x)^k = \frac{\Gamma\,(1+k)\,\Gamma\,(1+m)}{\Gamma\,(2+m+k)} \tag{C.7}$$

In the equation (C.6), yielding:[1]

$$I_{m,s} = \frac{\Gamma\,(1+s+m)\,\Gamma\,(1+s-m)}{\Gamma\,(2+2s)} = \frac{(s+m)!\,(s-m)!}{(2s+1)!}$$

If we apply the last result to the original expression for the closure relation, we get:

$$\left(\frac{2s+1}{4\pi}\right)\int_{S^2} d\Omega\,|\Omega^s\rangle\,\langle\Omega^s| = (2s+1)\sum_{m=-s}^{s}\frac{1}{2s+1}\,|s,m\rangle\,\langle s,m| = \mathbb{I}$$

Which is the result (3.13) that we were seeking.

[1]Note that the Gamma Function has the property $\Gamma\,(n) = (n-1)!$, when $n \in \mathbb{N}$.

C.4. Representations in the Spin Coherent State Basis and Kutzner's Theorem

Here, we wish to clarify the origin of the important expressions — (3.19)-(3.24) — as well as to prove that any operator can be written in diagonal form, using the basis of Spin Coherent-States.

C.4.1. Complex Plane Representation of Spin Coherent States

For these purposes, we start by recognizing that it is possible to represent a spin coherent-state by a complex number z, instead of a pair of angles (θ, ϕ). This mapping is done by the usual **stereographic projection** onto the equatorial plane (See [Figure C.1.]), yielding:

$$(\theta, \phi) \longmapsto z = e^{i\phi} \tan \frac{\theta}{2} \tag{C.8}$$

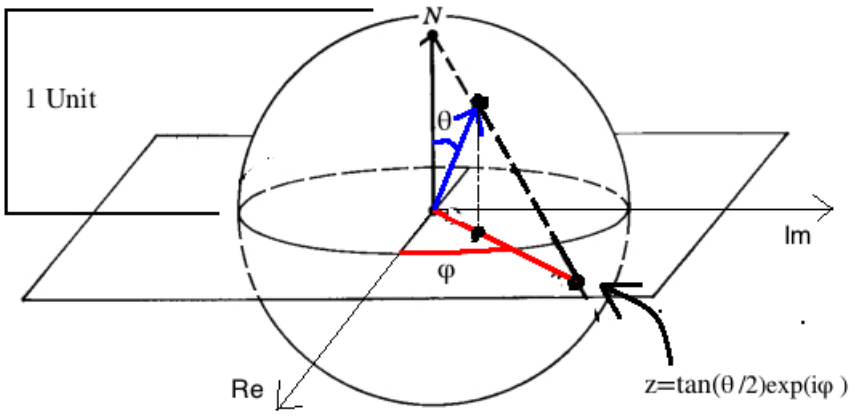


Figure C.1.: Scheme for the Stereographic Projection Mapping that allows a complex representation for the Spin Coherent States.

This change of variables also changes the integration measure in the closure relation (3.13), since $d^2z = \rho d\rho d\phi = \tan\theta/2 d\left(\tan\theta/2\right) d\phi = 1/4 \left(1 + \tan^2\theta/2\right)^2 \sin\theta d\theta d\phi$. Therefore, we have:

$$\frac{2s+1}{\pi} \int_{\mathbb{C}} \frac{d^2z}{\left(1+|z|^2\right)^2} |z^s\rangle \langle z^s| = \mathbb{I}^s$$

In the same way, we can write the expansion of a coherent state $\left|\hat{\Omega}^s\right\rangle$, in terms of $|s, m\rangle$ states using

the z parameter, instead of the Euler angles. This goes as follows:

$$\begin{aligned}
\left|\hat{\Omega}^s\right\rangle &= \sqrt{(2s)!}\sum_{m=-s}^{+s}\frac{u^{s+m}v^{s-m}}{\sqrt{(s+m)!\,(s-m)!}}\,|s,m\rangle = \\
&= \sqrt{(2s)!}\sum_{m=-s}^{+s}\frac{(\cos\theta/2\sin\theta/2)^s\,(\tan\theta/2)^{-m}\,e^{-im\phi}}{\sqrt{(s+m)!\,(s-m)!}}\,|s,m\rangle = \\
&= \sqrt{(2s)!}\sum_{m=-s}^{+s}\frac{|z|^{-m}\,e^{-im\phi}}{\sqrt{(s+m)!\,(s-m)!}}\left[\frac{1}{\left(1+|z|^2\right)\left(1+|z|^{-2}\right)}\right]^{s/2}|s,m\rangle = \\
&= e^{-is\phi}\sqrt{(2s)!}\sum_{m=-s}^{+s}\frac{|z|^{s-m}\,e^{i(s-m)\phi}}{\sqrt{(s+m)!\,(s-m)!}}\left[\frac{1}{\left(1+|z|^2\right)}\right]^{s}|s,m\rangle = \\
&= \frac{1}{\left(1+|z|^2\right)^s}e^{-is\phi}\sqrt{(2s)!}\sum_{m=-s}^{+s}\frac{z^{s-m}}{\sqrt{(s+m)!\,(s-m)!}}\,|s,m\rangle
\end{aligned} \tag{C.9}$$

Up to an irrelevant global phase factor[2], we get the expression:[3]

$$|\Omega^s\rangle \equiv |z^s\rangle = \frac{1}{\left(1+|z|^2\right)^s}\sqrt{(2s)!}\sum_{m=-s}^{+s}\frac{z^{s-m}}{\sqrt{(s+m)!\,(s-m)!}}\,|s,m\rangle \tag{C.10}$$

The overlap function can also be rewritten in terms of the complex parameter z:

$$\begin{aligned}
\langle z_1^s \mid z_2^s\rangle &= \frac{(2s)!}{\left(1+|z_1|^2\right)^s\left(1+|z_2|^2\right)^s}\sum_{m_1=-s}^{s}\sum_{m_2=-s}^{s}\frac{(z_1^*)^{s-m_1}\,z_2^{s-m_2}}{\sqrt{(s+m_1)!\,(s-m_1)!\,(s+m_2)!\,(s-m_2)!}}\delta_{m_1,m_2} = \\
&= \frac{(2s)!}{\left(1+|z_1|^2\right)^s\left(1+|z_2|^2\right)^s}\sum_{m=-s}^{s}\frac{(z_1^*z_2)^{s-m}}{(s+m)!\,(s-m)!} = \\
&= \frac{1}{\left(1+|z_1|^2\right)^s\left(1+|z_2|^2\right)^s}\sum_{k=0}^{2s}\binom{2s}{k}(z_1^*z_2)^{2s-k} = \frac{(1+z_1^*z_2)^{2s}}{\left(1+|z_1|^2\right)^s\left(1+|z_2|^2\right)^s}
\end{aligned} \tag{C.11}$$

C.4.2. Proof of Kutzner's Theorem on the Representation of Operators in the Coherent-State Basis

Now, we will use this complex representation for the spin coherent-states, to prove the referred **Kutzner's Theorem** [15,16], which can be stated as follows:

[2] This phase factor can be removed if one chooses the non-uniform gauge $\chi = -\phi$.

[3] In Refs [12,13,17,20,21] this is the way the authors define the spin coherent states, in the first place.
In Ref [12], the definition used for the state $|z^s\rangle$ is the following:

$$|z^s\rangle = \frac{1}{\left(1+|z|^2\right)^s}\exp(zS^-)\,|s,s\rangle$$

Which is seen to be equivalent to (C.10).

Theorem (Kutzner):

In terms of of the basis of spin coherent states $|z^s\rangle$, any linear operator A acting on the Hilbert Space of a spin-s system, can be given a diagonal representation as follows:

$$A = \frac{2s+1}{\pi}\int\int \frac{d^2z}{\left(1+|z|^2\right)^2} Tr\left[A\cdot\Delta_s\right]|z^s\rangle\langle z^s|$$

Where Δ_s is called the mapping operator, and is defined as:

$$\Delta_s(z) = \frac{(-1)^{2s}}{(2s+1)!}\sum_{m_1,m_2=-s}^{s}|s,m_1\rangle\langle s,m_2|\sqrt{\frac{(s-m_1)!(s+m_1)!}{(s-m_2)!(s+m_2)!}}(z*)^{m_1-m_2}\times$$
$$\times\sum_{k=0}^{s+m_1}\sum_{r=0}^{s-m_1}(-1)^{k+r}\begin{pmatrix} s+m_2 \\ s+m_1-k\end{pmatrix}\begin{pmatrix} s-m_2 \\ s-m_1-r\end{pmatrix}\frac{(2s+1+k+r)!}{r!k!}\frac{|z|^{2r}}{(1+|z|^2)^{k+r}}$$

a

[a] Note that both of these expressions reduce to (3.1.18-19), once we set $z=\tan\theta/2e^{i\phi}$ and $\frac{4d^2z}{\left(1+|z|^2\right)^2}=d\Omega$.

The proof of this theorem follows Ref. [15] and starts by showing the following equality:

$$I_{m,n}\equiv\frac{2s+1}{\pi}\int\int\frac{d^2z}{\left(1+|z|^2\right)^2}\langle s,m|\Delta_s(z)|s,n\rangle|z^s\rangle\langle z^s| = |s,n\rangle\langle s,m| \tag{C.12}$$

The matrix elements of the mapping operator — $\Delta_s(z)$ — are:

$$\langle s,m|\Delta_s(z)|s,n\rangle = \frac{(-1)^{2s}}{(2s+1)!}\sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}(z*)^{m-n}\times$$
$$\times\sum_{k=0}^{s+m}\sum_{r=0}^{s-m}(-1)^{k+r}\begin{pmatrix} s+n \\ s+m-k\end{pmatrix}\begin{pmatrix} s-n \\ s-m-r\end{pmatrix}\frac{(2s+1+k+r)!}{r!k!}\frac{|z|^{2r}}{(1+|z|^2)^{k+r}} \tag{C.13}$$

We can also use the definition of the states $|z^s\rangle$ in terms of standard spin states, to write:

$$|z^s\rangle\langle z^s| = \frac{1}{\left(1+|z|^2\right)^{2s}}(2s)!\sum_{j,l=-s}^{+s}\frac{(z^*)^{s-l}z^{s-j}}{\sqrt{(s+j)!(s-j)!(s+l)!(s-l)!}}|s,j\rangle\langle s,l| = \tag{C.14}$$

Placing (C.13) and (C.14) in (C.12), one ends up with the following scary expression:

$$I_{m,n} = \frac{(-1)^{2s}}{\pi}\sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\sum_{k=0}^{s-m}\sum_{r=0}^{s+m}\sum_{j,l=-s}^{+s}(-1)^{k+r}\left(\begin{array}{c} s+n \\ s+m-k \end{array}\right)\left(\begin{array}{c} s-n \\ s-m-r \end{array}\right)\frac{(2s+1+k+r)!}{r!k!}\times$$
$$\times\frac{|s,j\rangle\langle s,l|}{\sqrt{(s+j)!\,(s-j)!\,(s+l)!\,(s-l)!}}\int\int_{\mathbb{C}} d^2z\left[\frac{(z^*)^{m-n+s-l+r}\,z^{s-j+r}}{(1+|z|^2)^{2s+k+r+2}}\right] \tag{C.15}$$

Fortunately, the integral above can be done in a delightfully simple manner. Let us take the following standard integral:

$$J_{j,k,m} = \int\int d^2z\frac{z^j\,(z^*)^k}{\left(1+|z|^2\right)^{2+m}} = \int_0^\infty d\,|z|\,\frac{|z|^{j+k+1}}{\left(1+|z|^2\right)^{2+m}}\int_0^{2\pi} d\varphi e^{i(j-k)\varphi}$$

By symmetry, it is clear that $J_{j,k,m} = 0$ for the case where $j \neq k$. When $j = k$, we can make the change of variables — $z = \tan\theta/2 e^{i\phi}$ — and write the following:

$$\begin{aligned} J_{j,j,m} &= 1/4\int_0^{2\pi} d\phi\int_0^\pi \sin\theta d\theta\frac{\tan^{2k}\theta/2}{(1+\tan^2\theta/2)^m} = \pi/2\int_0^\pi \sin\theta d\theta\left(\cos^2\theta/2\right)^{m-k}\left(\sin^2\theta/2\right)^k = \\ &= \pi/2\int_0^\pi \sin\theta d\theta\left(\frac{1+\cos\theta}{2}\right)^{m-k}\left(\frac{1-\cos\theta}{2}\right)^k = \\ &= \pi\int_0^1 dx\,(1-x)^k\,x^{m-k} = \pi\frac{k!\,(m-k)!}{(m+1)!} \end{aligned} \tag{C.16}$$

In the last line of (C.16), we recognized the integral as being (C.7) of the [Appendix C.3.]. Applying (C.16) to the expression for $I_{m,n}$, we get:

$$I_{m,n} = (-1)^{2s}\sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\sum_{k=0}^{s+m}\sum_{r=0}^{s-m}\sum_{j,l=-s}^{+s}(-1)^{k+r}\begin{pmatrix} s+n \\ s+m-k \end{pmatrix}\begin{pmatrix} s-n \\ s-m-r \end{pmatrix}\frac{(2s+1+k+r)!}{r!k!}\times$$
$$\times\frac{|s,j\rangle\langle s,l|}{\sqrt{(s+j)!\,(s-j)!\,(s+l)!\,(s-l)!}}\frac{(s-j+r)!\,(s+k+j)!}{(s-j+r+1)!}\delta_{n-m+l,j} =$$

$$= (-1)^{2s}\sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\sum_{k=0}^{s+m}\sum_{r=0}^{s-m}\sum_{l=-s}^{+s}(-1)^{k+r}\begin{pmatrix} s+n \\ s+m-k \end{pmatrix}\begin{pmatrix} s-n \\ s-m-r \end{pmatrix}\frac{(2s+1+k+r)!}{r!k!}\times$$
$$\times\frac{|s,j\rangle\langle s,l|}{\sqrt{(s+n-m+l)!\,(s-n+m-l)!\,(s+l)!\,(s-l)!}}\frac{(s+j+r)!\,(s+k-j)!}{(2s+k+r+1)!}\delta_{n-m+l,j} =$$

$$= (-1)^{2s}\sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\sum_{l=-s}^{+s}\left[\sum_{k=0}^{s+m}(-1)^{k}\begin{pmatrix} s+n \\ s+m-k \end{pmatrix}\frac{(s+n-m+l+k)!}{k!}\right]\times$$
$$\left[\sum_{r=0}^{s-m}(-1)^{r}\begin{pmatrix} s-n \\ s-m-r \end{pmatrix}\frac{(s+m-n-l+r)!}{r!}\right]\frac{|s,n-m+l\rangle\langle s,l|}{\sqrt{(s+n-m+l)!\,(s-n+m-l)!\,(s+l)!\,(s-l)!}} \tag{C.17}$$

To do the sums inside brackets, we just have to use the following identity (which will be proven later in this Appendix):

$$\sum_{r=0}^{N}(-1)^{r}\begin{pmatrix} k \\ N-r \end{pmatrix}\frac{(n+r)!}{r!} = n!\begin{pmatrix} k-n-1 \\ N \end{pmatrix} \tag{C.18}$$

Applying this to (C.17), we get the intended result:

$$I_{m,n} = (-1)^{2s}\sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\sum_{l=-s}^{+s}\begin{pmatrix} l-m-1 \\ s-m \end{pmatrix}\begin{pmatrix} m-l-1 \\ s+m \end{pmatrix}$$
$$\times\frac{(s-m+n+l)!\,(s+m-n-l)!\,|s,n-m+l\rangle\langle s,l|}{\sqrt{(s+n-m+l)!\,(s-n+m-l)!\,(s+l)!\,(s-l)!}} =$$

$$= \sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\sum_{l=-s}^{+s}\delta_{m,l}\frac{(s-m+n+l)!\,(s+m-n-l)!\,|s,n-m+l\rangle\langle s,l|}{\sqrt{(s+n-m+l)!\,(s-n+m-l)!\,(s+l)!\,(s-l)!}} =$$

$$= \sqrt{\frac{(s-m)!(s+m)!}{(s-n)!(s+n)!}}\frac{(s+n)!\,(s-n)!\,|s,n\rangle\langle s,m|}{\sqrt{(s+n)!\,(s-n)!\,(s+m)!\,(s-m)!}} = |s,n\rangle\langle s,m|$$

Where in the first equality, we made use of the following fact:

$$\begin{pmatrix} k-n-1 \\ s+k \end{pmatrix} \begin{pmatrix} n-k-1 \\ s-k \end{pmatrix} = (-1)^{2s}\delta_{k,n} \tag{C.19}$$

- **Proof:**

This last expression is easily seen to be true, once we define, for $n, k \geq 0$ the following:

$$\begin{pmatrix} n \\ k \end{pmatrix} = 0,\ if\ k > n \quad and \quad \begin{pmatrix} -n \\ k \end{pmatrix} = \frac{(-n)\,(-n-1)\,...\,(-n-k+1)}{k!}$$

Given this, we see that for — $s \geq k > n \geq -s \Rightarrow s+k > k-n$ — meaning that $\begin{pmatrix} k-n-1 \\ s+k \end{pmatrix} = 0$.

On the other hand, for $s \geq n > k \geq -s$, we have $\begin{pmatrix} n-k-1 \\ s-k \end{pmatrix} = 0$.

The only non-zero case is then $n = k$, which yields:

$$\begin{pmatrix} -1 \\ s+k \end{pmatrix} \begin{pmatrix} -1 \\ s-k \end{pmatrix} = \frac{(-1)\,...(-s-k)}{(s+k)!}\frac{(-1)...(-s+k)}{(s-k)!} = (-1)^{2s}$$

Now that we have established that — $I_{m,n} = |s,n\rangle\langle s,m|$ — we can cast this equation in a slightly different shape, as follows:

$$\begin{aligned} |s,n\rangle\langle s,m| &= \frac{2s+1}{\pi}\int\int \frac{d^2z}{\left(1+|z|^2\right)^2}\langle s,m|\,\Delta_s(z)\,|s,n\rangle\,|z^s\rangle\langle z^s| = \\ &= \frac{2s+1}{\pi}\int\int \frac{d^2z}{\left(1+|z|^2\right)^2}\sum_{j=-s}^{s}\{\langle s,j\mid s,n\rangle\langle s,m|\,\Delta_s(z)\,|s,j\rangle\}\,|z^s\rangle\langle z^s| = \\ &= \frac{2s+1}{\pi}\int\int \frac{d^2z}{\left(1+|z|^2\right)^2} Tr\left\{|s,n\rangle\langle s,m|\,\Delta_s(z)\right\}|z^s\rangle\langle z^s| \end{aligned}$$

Where we made use of the fact that the standard basis is orthonormal — $\langle s,j \mid s,k\rangle = \delta_{j,k}$. The final step to prove Kutzner's Theorem is to expand an arbitrary operator A in terms of the basis $|s,m\rangle$ and finally use the above expression for the basis of linear operators — $|s,i\rangle\langle s,j|$. I.e.:

$$
\begin{aligned}
A &= \sum_{i,j=-s}^{s} \langle s,i|\, A\, |s,j\rangle\, |s,i\rangle\, \langle s,j| = \\
&= \frac{2s+1}{\pi} \int\int \frac{d^2z}{\left(1+|z|^2\right)^2} \sum_{i,j,k=-s}^{s} \left\{ \langle s,i|\, A\, |s,j\rangle\, \langle s,k \mid s,i\rangle\, \langle s,j|\, \Delta_s(z)\, |s,k\rangle \right\} |z^s\rangle\, \langle z^s| = \\
&= \frac{2s+1}{\pi} \int\int \frac{d^2z}{\left(1+|z|^2\right)^2} Tr\left\{ A \cdot \Delta_s(z) \right\} |z^s\rangle\, \langle z^s|
\end{aligned}
$$

Q.E.D.

Proof of the Identity (C.18):

The identity (C.18) can be readily proven by identifying it as an Hypergeometric Series. In fact, the following is true:

$$
\begin{aligned}
\sum_{r=0}^{N} (-1)^r \begin{pmatrix} k \\ N-r \end{pmatrix} \frac{(n+r)!}{r!} x^r &= n! \begin{pmatrix} k \\ N \end{pmatrix} \sum_{r=0}^{N} (-1)^r \begin{pmatrix} N \\ r \end{pmatrix} \times \frac{(k-N)!\,(n+r)!}{n!\,(k+r-N)!} \times x^r = \\
&= n! \begin{pmatrix} k \\ N \end{pmatrix} F_1^2\left(-N, n+1, k-N+1, x\right)
\end{aligned}
$$

Where we made the identification of the last sum, with the series expansion for the Hypergeometric function (2F1) as a function of its last argument. In our special case — $x = 1$ — Gauss's Identity applies[4], yielding:

$$
F_1^2\left(-N, n+1, k-N+1, 1\right) = \frac{\Gamma(k-N+1)}{\Gamma(k+1)} \frac{\Gamma(k-n)}{\Gamma(k-N-n)} = \frac{(k-N)!}{k!} \frac{(k-n-1)!}{(k-N-n-1)!}
$$

Plugging this result into the last expression for the sum over r, we get:

$$
\begin{aligned}
\sum_{r=0}^{N} (-1)^r \begin{pmatrix} k \\ N-r \end{pmatrix} \frac{(n+r)!}{r!} &= \frac{n!k!}{N!(k-N)!} \frac{(k-N)!(k-n-1)!}{k!(k-N-n-1)!} = \\
&= n! \frac{(k-n-1)!}{N!(k-N-n-1)!} = n! \begin{pmatrix} k-n-1 \\ N \end{pmatrix}
\end{aligned}
$$

And thus, we prove the identity.

[4] Strictly speaking, this only applies in the case when $n < k$, but once we extend the binomial coefficients to negative upper arguments, as we've done previously, the final result still holds.

C.4.3. Representation of the Spin Components in the Basis of Coherent States

As an illustrative application and also for future use, we proceed with the calculation of the diagonal representation for the spin operators $S^{\pm}$ and S^z. To do that we only need to calculate the traces of these operators multiplied by the mapping operator — $\Delta_s(z)$. Remembering the relations (1.7):

$$S^{\pm}\left|s,m_s\right\rangle = \sqrt{s(s+1)-m_s(m_s\pm 1)}\left|s,m_s\pm 1\right\rangle, \quad S^z\left|s,m_s\right\rangle = m_s\left|s,m_s\right\rangle$$

Therefore, we get the following formal expressions:

$$\begin{aligned} Tr[S^z\Delta_s] = \frac{(-1)^{2s}}{(2s+1)!}\sum_{J=-s}^{s} J\sum_{k=0}^{s+J}\sum_{r=0}^{s-J}(-1)^{k+r}\left(\begin{array}{c} s+J \\ s+J-k \end{array}\right)\left(\begin{array}{c} s-J \\ s-J-r \end{array}\right)\times \\ \times\frac{(2s+1+k+r)!}{r!k!}\frac{|z|^{2r}}{(1+|z|^2)^{k+r}} \end{aligned} \tag{C.20}$$

$$\begin{aligned} Tr[S^+\Delta_s] = \frac{(-1)^{2s}}{(2s+1)!}\sum_{J=-s}^{s-1}\sqrt{s(s+1)-J(J+1)}\sqrt{\frac{(s-J)!(s+J)!}{(s-J-1)!(s+J+1)!}}\,(z*)^{-1}\times \\ \times\sum_{k=0}^{s+J}\sum_{r=0}^{s-J}(-1)^{k+r}\left(\begin{array}{c} s+J+1 \\ s+J-k \end{array}\right)\left(\begin{array}{c} s-J-1 \\ s-J-r \end{array}\right)\frac{(2s+1+k+r)!}{r!k!}\frac{|z|^{2r}}{(1+|z|^2)^{k+r}} \end{aligned} \tag{C.21}$$

$$\begin{aligned} Tr[S^-\Delta_s] = \frac{(-1)^{2s}}{(2s+1)!}\sum_{J=-s+1}^{s}\sqrt{s(s+1)-J(J-1)}\sqrt{\frac{(s-J)!(s+J)!}{(s-J+1)!(s+J-1)!}}\,(z*)\times \\ \times\sum_{k=0}^{s+J}\sum_{r=0}^{s-J}(-1)^{k+r}\left(\begin{array}{c} s+J-1 \\ s+J-k \end{array}\right)\left(\begin{array}{c} s-J+1 \\ s-J-r \end{array}\right)\frac{(2s+1+k+r)!}{r!k!}\frac{|z|^{2r}}{(1+|z|^2)^{k+r}} \end{aligned} \tag{C.22}$$

These three expressions were programmed on a Mathematica notebook, which produced the following simple expressions:

$$Tr[S^z\Delta_s] = (s+1)\,\frac{1-|z|^2}{1+|z|^2} \tag{C.23}$$

$$Tr[S^+\Delta_s] = (s+1)\,\frac{2z}{1+|z|^2} \tag{C.24}$$

$$Tr[S^-\Delta_s] = (s+1)\,\frac{2z^*}{1+|z|^2} \tag{C.25}$$

Finally, we can make the replacement — $z = \tan\theta/2 e^{i\phi}$ — and express the spin components in terms of the original (θ,ϕ) parameters, getting:

$$S^x = {}^1\!/_2 \left(S^+ + S^-\right) = \frac{(2s+1)(s+1)}{\pi} \int\int \frac{d^2z}{\left(1+|z|^2\right)^2} \frac{z+z^*}{1+|z|^2} |z^s\rangle \langle z^s| =$$
$$= \frac{(2s+1)(s+1)}{4\pi} \int d\Omega \sin\theta \cos\phi \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{C.26}$$

$$S^y = {}^i\!/_2 \left(S^- - S^+\right) = \frac{i\,(2s+1)(s+1)}{\pi} \int\int \frac{d^2z}{\left(1+|z|^2\right)^2} \frac{z^*-z}{1+|z|^2} |z^s\rangle \langle z^s| =$$
$$= \frac{(2s+1)(s+1)}{4\pi} \int d\Omega \sin\theta \sin\phi \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{C.27}$$

$$S^z = \frac{(2s+1)(s+1)}{\pi} \int\int \frac{d^2z}{\left(1+|z|^2\right)^2} \frac{1-|z|^2}{1+|z|^2} |z^s\rangle \langle z^s| =$$
$$= \frac{(2s+1)(s+1)}{4\pi} \int d\Omega \cos\theta \left|\hat{\Omega}^s\right\rangle \left\langle\hat{\Omega}^s\right| \tag{C.28}$$

Which are the results quoted in equations (3.19-22). In the same way, the above equations can be used to calculate the expectation values for the spin components, in any coherent-state, as follows:

$$\left\langle\hat{\Omega}^s\right| S^x \left|\hat{\Omega}^s\right\rangle = \frac{(2s+1)(s+1)}{4\pi} \int_0^\pi d\theta' \int_0^{2\pi} d\phi' \sin^2\theta \cos\phi \left|\langle\theta,\phi \mid \theta',\phi'\rangle\right|^2 =$$
$$= \frac{(2s+1)(s+1)}{4\pi} \int_{-1}^1 dx \int_0^{2\pi} dy \sqrt{1-x^2} \cos y \left({}^1\!/_2 \left(1 + x\cos(\theta) + \sqrt{1-x^2}\sin\theta\cos(y-\phi)\right)\right)^{2s} \tag{C.29}$$

$$\left\langle\hat{\Omega}^s\right| S^y \left|\hat{\Omega}^s\right\rangle = \frac{(2s+1)(s+1)}{4\pi} \int_0^\pi d\theta' \int_0^{2\pi} d\phi' \sin^2\theta \sin\phi \left|\langle\theta,\phi \mid \theta',\phi'\rangle\right|^2 =$$
$$= \frac{(2s+1)(s+1)}{4\pi} \int_{-1}^1 dx \int_0^{2\pi} dy \sqrt{1-x^2} \sin y \left({}^1\!/_2 \left(1 + x\cos(\theta) + \sqrt{1-x^2}\sin\theta\cos(y-\phi)\right)\right)^{2s} \tag{C.30}$$

$$\left\langle\hat{\Omega}^s\right| S^z \left|\hat{\Omega}^s\right\rangle = \frac{(2s+1)(s+1)}{4\pi} \int_0^\pi d\theta' \int_0^{2\pi} d\phi' \sin\theta\cos\theta \left|\langle\theta,\phi \mid \theta',\phi'\rangle\right|^2 =$$
$$= \frac{(2s+1)(s+1)}{4\pi} \int_{-1}^1 dx \int_0^{2\pi} dy x \left({}^1\!/_2 \left(1 + x\cos(\theta) + \sqrt{1-x^2}\sin\theta\cos(y-\phi)\right)\right)^{2s} \tag{C.31}$$

These integrals are very hard to do and we could not calculate them by hand. However, we managed to verify them for the cases $s = \{1/2, ..., 3\}$ (using the symbolic calculation capabilities of Mathematica)

and concluded that they yield the results that are expected, knowing that $\left|\hat{\Omega}\right\rangle$ is the highest-spin projection state with respect to the spin component operator, along the axis (θ, ϕ). I.e.:

$$\left\langle \hat{\Omega}^s \right| S^x \left| \hat{\Omega}^s \right\rangle = s \sin\theta \cos\phi; \quad \left\langle \hat{\Omega}^s \right| S^y \left| \hat{\Omega}^s \right\rangle = s \sin\theta \cos\phi; \quad \left\langle \hat{\Omega}^s \right| S^z \left| \hat{\Omega}^s \right\rangle = s \cos\theta \tag{C.32}$$

C.4.4. General Proof for the Expectation Values of Spin Operators in the Coherent-State Basis

A general and more manageable way of obtaining (C.32), is to calculate directly the averages of $S^{\pm}$ and S^z, using the expression (C.10) for the coherent-states. We start by rewriting (C.10), as follows:

$$|z^s\rangle = \frac{z^{2s}}{\left(1+|z|^2\right)^s} \sum_{p=0}^{2s} \left[\frac{(2s)!}{p!(2s-p)!}\right]^{1/2} z^{-p} \, |p\rangle \quad \text{with } |p\rangle \equiv |s, p-s\rangle \tag{C.33}$$

Starting from the case $\hat{P} = S^z + s$, we have — $\hat{P}\,|p\rangle = p\,|p\rangle$ — and hence[5]:

$$\begin{aligned} \langle z^s| \, \hat{P} \, |z^s\rangle &= \frac{|z|^{4s}}{\left(1+|z|^2\right)^{2s}} \sum_{p_1,p_2=0}^{2s} \frac{(2s)!}{\sqrt{p_1!(2s-p_1)!p_2!(2s-p_2)!}} z^{-p_1} \left(z^*\right)^{-p_2} p_1 \, \langle p_2 \mid p_1\rangle = \\ &= \frac{|z|^{4s}}{\left(1+|z|^2\right)^{2s}} \sum_{p=1}^{2s} \frac{(2s)!}{p!(2s-p)!} \, |z|^{-2p} \, p = \frac{2s}{1+|z|^2} \end{aligned} \tag{C.34}$$

Which can be turned into the following:

$$\langle z^s| \, S^z \, |z^s\rangle = s \frac{1-|z|^2}{1+|z|^2} = s\cos\theta \tag{C.35}$$

The same procedure can be applied to the expectation values of the ladder operators — $S^{\pm}$ — starting from the fact that — $S^- \, |p\rangle = \sqrt{p(2s-p+1)} \, |p-1\rangle$— and using the definition (C.33):

[5] To perform the last sum in (C.34), we have used the fact that:

$$\sum_{k=1}^{2s} \frac{(2s)!}{k!(2s-k)!} k x^k = x \frac{\partial}{\partial x} \left[\sum_{k=0}^{2s} \frac{(2s)!}{k!(2s-k)!} x^k \right] = x \frac{\partial}{\partial x} (1+x)^{2s} = 2sx(1+x)^{2s-1}$$

$$\begin{aligned}
\langle z^s|\, S^- \,|z^s\rangle &= \frac{|z|^{4s}}{\left(1+|z|^2\right)^{2s}} \sum_{p_1,p_2=0}^{2s} \frac{(2s)!\sqrt{p_1(2s-p_1+1)}}{\sqrt{p_1!(2s-p_1)!p_2!(2s-p_2)!}} z^{-p_1} \left(z^*\right)^{-p_2} \langle p_2 \mid p_1-1\rangle = \\
&= \frac{|z|^{4s}}{\left(1+|z|^2\right)^{2s}} \sum_{p=1}^{2s} \frac{(2s)!\sqrt{p(2s-p+1)}}{\sqrt{p!(2s-p)!(p-1)!(2s-p+1)!}} z^{-p} \left(z^*\right)^{-p+1} = \\
&= \frac{|z|^{4s}}{\left(1+|z|^2\right)^{2s}} \sum_{p=1}^{2s} \frac{(2s)!}{(p-1)!(2s-p)!} z^{-p} \left(z^*\right)^{-p+1} = \\
&= \frac{z^*\,|z|^{4s}}{\left(1+|z|^2\right)^{2s}} \sum_{p=1}^{2s} \frac{(2s)!}{(p)!(2s-p)!} p\,|z|^{-2p} = \frac{2sz^*}{1+|z|^2}
\end{aligned} \tag{C.36}$$

Consequently, we also have:

$$\langle z^s|\, S^+ \,|z^s\rangle = \langle z^s|\, S^- \,|z^s\rangle^* = \frac{2sz}{1+|z|^2} \tag{C.37}$$

Using (C.36) and (C.37), we can obtain the expression for the expectation values of S^x and S^y, as follows:

$$\begin{aligned}
\langle z^s|\, S^x \,|z^s\rangle &= \frac{1}{2}\left[\langle z^s|\, S^+ \,|z^s\rangle + \langle z^s|\, S^- \,|z^s\rangle\right] = s\frac{z+z^*}{1+|z|^2} = \\
&= s\frac{\tan\theta/2}{1+\tan^2\theta/2}\left(e^{i\phi}+e^{-i\phi}\right) = 2s\sin\theta/2\cos\theta/2\cos\phi = \\
&= s\sin\theta\cos\phi
\end{aligned} \tag{C.38}$$

$$\begin{aligned}
\langle z^s|\, S^y \,|z^s\rangle &= \frac{i}{2}\left[\langle z^s|\, S^- \,|z^s\rangle - \langle z^s|\, S^+ \,|z^s\rangle\right] = is\frac{z^*-z}{1+|z|^2} = \\
&= 2s\frac{\tan\theta/2}{1+\tan^2\theta/2} i\left(e^{-i\phi}-e^{i\phi}\right) = 2s\sin\theta/2\cos\theta/2\sin\phi = \\
&= s\sin\theta\sin\phi
\end{aligned} \tag{C.39}$$

And these two results are precisely the ones obtained in (C.32), but now proven to be true for any value of s.

C.5. Derivation of the Correlation Functions from a Generating Functional

In this short Appendix, we wish to demonstrate directly how one can obtain the averages (3.37) and (3.38) from the general functional $Z[J(\tau)]$. To do that, we just have to remember the basic properties

of functional derivatives for (bosonic) functionals, which are well given in any Quantum Field Theory (e.g. Ref. [22]), and go as follows:

$$\frac{\delta}{\delta F(x)}F(y)=\delta^{(d)}(x-y);\quad \frac{\delta}{\delta F(x)}\int d^dyF(y)G(y)=F(x)\ +\quad \text{(Linear and Liebnitz)}$$

These can be extended to the derivative of any analytic function of a functional integral [such as the exponential] simply by formally expanding it into a Taylor series and using the above rules on each of the terms. We get then:

$$\frac{\delta}{\delta F(x)}\exp\left\{i\int d^dyF(y)G(y)\right\}=iG(x)\exp\left\{i\int d^dyF(y)G(y)\right\}$$

Applying the above rule to the functional $Z[J(\tau)]$ given in (3.2.7), we get:

$$\begin{aligned}\frac{\delta}{\delta J_j^\beta(\tau')}Z[J(\tau)]&=Tr\left\{T_\tau\left[\frac{\delta}{\delta J_j^\beta(\tau')}\exp\left\{-\int_0^\beta d\tau\left(H_0+\sum_{i,\alpha}J_i^\alpha(\tau)S_i^\alpha(\tau)\right)\right\}\right]\right\}=\\&=Tr\left\{T_\tau\left[S_j^\beta(\tau')\exp\left\{-\int_0^\beta d\tau\left(H_0+\sum_{i,\alpha}J_i^\alpha(\tau)S_i^\alpha(\tau)\right)\right\}\right]\right\}\end{aligned}$$

Differentiating a second time:

$$\begin{aligned}\frac{\delta}{\delta J_k^\gamma(\tau'')}\frac{\delta}{\delta J_j^\beta(\tau')}Z[J(\tau)]&=Tr\left\{T_\tau\left[\frac{\delta}{\delta J_k^\gamma(\tau'')}S_j^\beta(\tau')\exp\left\{-\int_0^\beta d\tau\left(H_0+\sum_{i,\alpha}J_i^\alpha(\tau)S_i^\alpha(\tau)\right)\right\}\right]\right\}=\\&=Tr\left\{T_\tau\left[S_j^\beta(\tau')S_k^\gamma(\tau'')\exp\left\{-\int_0^\beta d\tau\left(H_0+\sum_{i,\alpha}J_i^\alpha(\tau)S_i^\alpha(\tau)\right)\right\}\right]\right\}\end{aligned}$$

By taking now the values of the above two derivatives at zero field, i.e. $J(\tau)=0$, and noticing that $\tau\in[0,\beta[$ we get the wanted results:

$$\frac{\delta}{\delta J_j^\beta(\tau')}Z[J(\tau)]\mid_{J=0}=Tr\left\{\exp\{-\beta H_0\}\,S_j^\beta(\tau')\right\}=\left\langle S_j^\beta(\tau)\right\rangle$$

$$\frac{\delta}{\delta J_k^\gamma(\tau'')}\frac{\delta}{\delta J_j^\beta(\tau')}Z[J(\tau)]\mid_{J=0}=Tr\left\{\exp\{-\beta H_0\}\,T_\tau\left[S_j^\beta(\tau')S_k^\gamma(\tau'')\right]\right\}=\left\langle\mathcal{T}_\tau\left[S_j^\beta(\tau')S_k^\gamma(\tau'')\right]\right\rangle$$

These results obviously generalize to any n-point correlation function of the system.

C.6. Can the Partition Function be Written as a Trace over Spin Coherent-States?

In this Appendix, we wish to show the expression (3.39), which states that it is possible to write the Generating Functional — $Z[J(\tau)]$ — as a trace in the non-orthogonal basis of spin coherent-states. For clarity, we remind the essential definition here (for a single site $i \in \mathscr{L}$):

$$\left|\hat{\Omega}_i^s\right\rangle = \frac{\left(ua_i^\dagger + vb_i^\dagger\right)^{2s}}{\sqrt{(2s)!}}\left|0\right\rangle_i = \sqrt{(2s)!}\sum_{m_i=-s}^{+s}\frac{u_i^{s-m_i}v_i^{s+m_i}}{\sqrt{(s+m_i)!\,(s-m_i)!}}\left|s,m_i\right\rangle. \tag{C.40}$$

With $u_i(\theta,\phi) = e^{-i\phi/2}\cos\theta/2$, $v_i(\theta,\phi) = e^{i\phi/2}\sin\theta/2$. The generalization of (C.40) to several spins is done by taking the tensor product of these states, i.e.:

$$\left|\Omega\right\rangle = \otimes_{i\in\mathscr{L}}\left|\hat{\Omega}_i^s\right\rangle. \tag{C.41}$$

The basis (C.40) has some important properties, that were proven in Chapter 3. The first is the fact that (C.40) is a non-orthogonal overcomplete set of vectors with the following overlap function:

$$\left\langle\hat{\Omega}_{1i}\mid\hat{\Omega}_{2i}\right\rangle = \left[\frac{1+\hat{\Omega}_{1i}\cdot\hat{\Omega}_{2i}}{2}\right]^s e^{i\sum_i\Psi(\hat{\Omega}_{1i},\hat{\Omega}_{2i})}, \tag{C.42}$$

for a phase function defined as:

$$\Psi(\hat{\Omega}_{1i},\hat{\Omega}_{2i}) \equiv 2s\arctan\left\{\tan\left(\frac{\phi_{2i}-\phi_{1i}}{2}\right)\frac{\cos\left(\frac{\theta_{1i}+\theta_{2i}}{2}\right)}{\cos\left(\frac{\theta_{1i}-\theta_{2i}}{2}\right)}\right\}.$$

Secondly, they obey a closure relation with an altered integration measure, in the Ω-sphere:

$$\mathbb{I}_i^s = \left(\frac{2s+1}{4\pi}\right)\int_{S^2} d\hat{\Omega}_i\left|\hat{\Omega}_i^s\right\rangle\left\langle\hat{\Omega}_i^s\right|. \tag{C.43}$$

And at last, we proved also that any operator A, acting on the Hilbert Space of a single spin-s, can be given a diagonal representation (Kutzner's Theorem), which goes as follows:

$$A = \left(\frac{2s+1}{4\pi}\right)\int d\hat{\Omega}_i\; a(\hat{\Omega}_i)\left|\hat{\Omega}_i^s\right\rangle\left\langle\hat{\Omega}_i^s\right|. \tag{C.44}$$

In order to use this new basis for representing the trace in (3.39), we need to prove that the trace of an arbitrary operator A is the same whether it is calculated in the basis $\left|\hat{\Omega}_i^s\right\rangle$ or in the original standard basis (which is orthonormal):

$$|\phi_{m_1,...,m_N}\rangle = \otimes_{i\in\mathscr{L}} |s, m_i\rangle \text{ with } m_i \in \{-s, -s+1, ..., s-1, s\}. \tag{C.45}$$

As remarked on a footnote of the main text, this equivalence is not obvious, since the new basis cannot be obtained from (C.45) by an unitary transformation (i.e. the coherent-states are not an orthonormal basis). However, starting with the case of a single spin and using the result (C.44), we can prove this result as follows:

$$\begin{aligned}
\mathrm{Tr}A_i &= \sum_{m_i=-s}^{s} \langle s, m_i| A_i |s, m_i\rangle = \\
&= \left(\frac{2s+1}{4\pi}\right) \int d\hat{\Omega}_i a(\hat{\Omega}_i) \sum_{m_i=-s}^{s} \langle s, m_i| \left|\hat{\Omega}_i^s\right\rangle \left\langle\hat{\Omega}_i^s\right| |s, m_i\rangle = \\
&= \left(\frac{2s+1}{4\pi}\right) \int d\hat{\Omega}_i a(\hat{\Omega}_i) \left\langle\hat{\Omega}_i^s\right| \sum_{m_i=-s}^{s} |s, m_i\rangle \langle s, m_i| \left|\hat{\Omega}_i^s\right\rangle = \qquad \text{(C.46)} \\
&= \left(\frac{2s+1}{4\pi}\right) \int d\hat{\Omega}_i a(\hat{\Omega}_i) \left\langle\hat{\Omega}_i^s\right| \mathbb{I}_i^s \left|\hat{\Omega}_i^s\right\rangle = \\
&= \left(\frac{2s+1}{4\pi}\right)^2 \int d\hat{\Omega}_i a(\hat{\Omega}_i) \left\langle\hat{\Omega}_i^s\right| \int d\hat{\Omega}_{2i} \left|\hat{\Omega}_{2i}^s\right\rangle \left\langle\hat{\Omega}_{2i}^s\right| \left|\hat{\Omega}_i^s\right\rangle = \qquad \text{(C.47)} \\
&= \left(\frac{2s+1}{4\pi}\right)^2 \int d\hat{\Omega}_i \int d\hat{\Omega}_{2i} a(\hat{\Omega}_i) \left\langle\hat{\Omega}_{2i}^s\right| \left|\hat{\Omega}_i^s\right\rangle \left\langle\hat{\Omega}_i^s\right| \left|\hat{\Omega}_{2i}^s\right\rangle = \\
&= \left(\frac{2s+1}{4\pi}\right) \int d\hat{\Omega}_{2i} \left\langle\hat{\Omega}_{2i}^s\right| \left\{ \left(\frac{2s+1}{4\pi}\right) \int d\hat{\Omega}_i a(\hat{\Omega}_i) \left|\hat{\Omega}_i^s\right\rangle \left\langle\hat{\Omega}_i^s\right| \right\} \left|\hat{\Omega}_{2i}^s\right\rangle = \qquad \text{(C.48)} \\
&= \left(\frac{2s+1}{4\pi}\right) \int d\hat{\Omega}_{2i} \left\langle\hat{\Omega}_{2i}^s\right| A_i \left|\hat{\Omega}_{2i}^s\right\rangle . \qquad \text{(C.49)}
\end{aligned}$$

In (C.46), we used the closure relation for the discrete basis $\{|s, m\rangle\}$, in (C.47) we replaced the identity operator by the closure relation (C.43) and, finally, in (C.48) we have identified the representation (C.44) for the local operator A_i, in terms of spin coherent-states.

In order to generalize this for a system of many spins, one starts by realizing that it is enough to prove it for an operator that can be written as a product of single-site operators A_i — like in (C.50). This is sufficient, because any operator can be written as a linear combination of operators of this type (e.g. any operator can be written in terms of the basis of projectors onto the product basis states).

$$A = \otimes_{i\in\mathscr{L}} A_i \tag{C.50}$$

Finally, we can calculate the trace of (C.50), yielding:

$$\begin{aligned}\mathrm{Tr}A &= \sum_{m_1,\ldots,m_N=-s}^{s} \langle \phi_{m_1,\ldots,m_N} | \, A \, | \phi_{m_1,\ldots,m_N} \rangle = \\ &= \sum_{m_1,\ldots,m_N=-s}^{s} \left\{ \prod_{i\in\mathscr{L}} \langle s, m_i | \, A_i \, | s, m_i \rangle \right\} = \\ &= \prod_{i\in\mathscr{L}} \left\{ \sum_{m_i=-s}^{s} \langle s, m_i | \, A_i \, | s, m_i \rangle \right\}. \end{aligned} \tag{C.51}$$

Using (C.49) into the expression (C.51), we arrive at the following final result:

$$\begin{aligned}\mathrm{Tr}A &= \prod_{i\in\mathscr{L}} \left\{ \left(\frac{2s+1}{4\pi} \right) \int d\hat{\Omega}_i \left\langle \hat{\Omega}_i^s \right| A_i \left| \hat{\Omega}_i^s \right\rangle \right\} = \\ &= \left(\frac{2s+1}{4\pi} \right)^N \left\{ \prod_{i\in\mathscr{L}} \int d\hat{\Omega}_i \right\} \langle \Omega | \otimes_{i\in\mathscr{L}} A_i \, | \Omega \rangle = \\ &= \left(\frac{2s+1}{4\pi} \right)^N \int d\Omega \, \langle \Omega | \, A \, | \Omega \rangle . \end{aligned} \tag{C.52}$$

At last, by choosing A to be the following operator:

$$A = T_\tau \left[\exp \left\{ - \int_0^\beta d\tau \left(H_0 + \sum_{k,\alpha} J_k^\alpha(\tau) S_k^\alpha(\tau) \right) \right\} \right]$$

And using (C.52), we can write the generating functional, written as we wanted:

$$Z[J(\tau)] = \left(\frac{2s+1}{4\pi} \right)^N \int d\Omega \, \langle \Omega | \, T_\tau \left[\exp \left\{ - \int_0^\beta d\tau \left(H_0 + \sum_{k,\alpha} J_k^\alpha(\tau) S_k^\alpha(\tau) \right) \right\} \right] | \Omega \rangle \tag{C.53}$$

C.7. Auxiliary Calculations For The Haldane Mapping

In this appendix, we wish to calculate explicitly both expression (3.74) and also the expansion of the Berry phase term in the spin action.

We start by writing the last term in (3.73), as a momentum-space integral, using the definitions given in [Appendix A.1]. Hence we have:

$$\sum_{i,j\in\mathscr{L}} J_{ij}\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_j-\frac{1}{2}\eta_i\eta_j\left[\overrightarrow{\mathbf{K}}_i\cdot\overrightarrow{\mathbf{K}}_i+\overrightarrow{\mathbf{K}}_j\cdot\overrightarrow{\mathbf{K}}_j\right]\right]=$$
$$=\sum_{\overrightarrow{\mathbf{p}},\overrightarrow{\mathbf{q}}_1,\overrightarrow{\mathbf{q}}_2} J_{\overrightarrow{\mathbf{p}}}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}_1}\cdot\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}_2}\sum_{i,j}\Big[e^{i\overrightarrow{\mathbf{x}}_i\cdot\left(\overrightarrow{\mathbf{q}}_2-\overrightarrow{\mathbf{p}}\right)}e^{i\overrightarrow{\mathbf{x}}_j\cdot\left(\overrightarrow{\mathbf{q}}_1+\overrightarrow{\mathbf{p}}\right)}-$$
$$-\frac{1}{2}e^{i\overrightarrow{\mathbf{x}}_i\cdot\left(\overrightarrow{\mathbf{q}}_1+\overrightarrow{\mathbf{q}}_2+\frac{\overrightarrow{\pi}}{a}-\overrightarrow{\mathbf{p}}\right)}e^{i\overrightarrow{\mathbf{x}}_j\cdot\left(\overrightarrow{\mathbf{p}}-\frac{\overrightarrow{\pi}}{a}\right)}-\frac{1}{2}e^{i\overrightarrow{\mathbf{x}}_j\cdot\left(\overrightarrow{\mathbf{q}}_1+\overrightarrow{\mathbf{q}}_2+\frac{\overrightarrow{\pi}}{a}-\overrightarrow{\mathbf{p}}\right)}e^{i\overrightarrow{\mathbf{x}}_i\cdot\left(\overrightarrow{\mathbf{p}}-\frac{\overrightarrow{\pi}}{a}\right)}$$

Using the fact that $\sum_j e^{i\overrightarrow{\mathbf{x}}_j\cdot\overrightarrow{\mathbf{q}}}=\delta_{\overrightarrow{\mathbf{q}},\overrightarrow{\mathbf{0}}}$, we can simplify the last expression as follows:

$$...=\sum_{\overrightarrow{\mathbf{p}},\overrightarrow{\mathbf{q}}_1,\overrightarrow{\mathbf{q}}_2} J_{\overrightarrow{\mathbf{p}}}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}_1}\cdot\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}_2}\left[\delta_{\overrightarrow{\mathbf{q}}_2,\overrightarrow{\mathbf{p}}}\delta_{-\overrightarrow{\mathbf{q}}_1,\overrightarrow{\mathbf{p}}}-\delta_{\overrightarrow{\mathbf{p}},\frac{\overrightarrow{\pi}}{a}}\delta_{\overrightarrow{\mathbf{q}}_1,-\overrightarrow{\mathbf{q}}_2}\right]=\sum_{\overrightarrow{\mathbf{p}}\in FBZ}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{p}}}\cdot\overrightarrow{\mathbf{K}}_{-\overrightarrow{\mathbf{p}}}\left[J(\overrightarrow{\mathbf{p}})-J(\frac{\overrightarrow{\pi}}{a})\right]=$$
$$=\int_{FBZ}\frac{d^D\overrightarrow{\mathbf{q}}}{(2\pi)^D}\chi^{-1}_{\overrightarrow{\mathbf{q}}}\overrightarrow{\mathbf{K}}_{\overrightarrow{\mathbf{q}}}\cdot\overrightarrow{\mathbf{K}}_{-\overrightarrow{\mathbf{q}}}$$

Which is precisely the wanted expression.

Secondly, we will obtain the functional derivative of the Berry phase functional, defined as:

$$\omega[\overrightarrow{\Omega}_i]=\int_0^\beta d\tau\,\overrightarrow{A}[\overrightarrow{\Omega}_i(\tau)]\cdot\frac{d}{d\tau}\overrightarrow{\mathbf{\Omega}}_i$$

A variation relative to $\overrightarrow{\mathbf{\Omega}}_i$ goes as follows (as usual, the variations are done with the end-points fixed, i.e. $\delta\Omega(0)=\delta\Omega(\beta)=0$):

$$\delta\omega[\overrightarrow{\Omega}_i]=\int_0^\beta d\tau\left(\delta\overrightarrow{A}[\overrightarrow{\Omega}_i(\tau)]\right)\cdot\frac{d}{d\tau}\overrightarrow{\mathbf{\Omega}}_i+\overrightarrow{A}[\overrightarrow{\Omega}_i(\tau)]\cdot\frac{d}{d\tau}\left(\delta\overrightarrow{\mathbf{\Omega}}_i\right)=$$
$$=\int_0^\beta d\tau\left[\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\delta\Omega^\beta\dot{\Omega}_\alpha+A^\alpha\frac{d}{d\tau}\left(\delta\Omega_\alpha\right)\right]$$

Now, we introduce the null term - $\int_0^\beta d\tau\left[\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\dot{\Omega}^\beta\delta\Omega_\alpha-\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\dot{\Omega}^\beta\delta\Omega_\alpha\right]$- for convenience. This allow us to re-write the above expression as:

$$\delta\omega[\overrightarrow{\Omega}_i]=\int_0^\beta d\tau\left[\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\delta\Omega^\beta\dot{\Omega}_\alpha-\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\dot{\Omega}^\beta\delta\Omega_\alpha+\frac{d}{d\tau}\left(A^\alpha\delta\Omega_\alpha\right)\right]=$$
$$=\int_0^\beta d\tau\left[\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\delta\Omega^\beta\dot{\Omega}_\alpha-\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\dot{\Omega}^\beta\delta\Omega_\alpha\right]+\int_0^\beta d\tau\left[\frac{d}{d\tau}\left(A^\alpha\delta\Omega_\alpha\right)\right]=$$
$$=\int_0^\beta d\tau\left[\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\delta\Omega^\beta\dot{\Omega}_\alpha-\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\dot{\Omega}^\beta\delta\Omega_\alpha\right]=$$
$$=\int_0^\beta d\tau\left[\left(\frac{\partial A^\alpha}{\partial\Omega^\beta}\right)\epsilon^{\alpha\beta\gamma}\epsilon^{\gamma\mu\nu}\dot{\Omega}_\mu\delta\Omega_\nu\right]=\int_0^\beta d\tau\left[\left(\overrightarrow{\nabla}\times\overrightarrow{\mathbf{A}}\right)^\gamma\left(\dot{\Omega}\times\delta\Omega\right)_\gamma\right]$$

Finally, from (3.54), we know that $\overrightarrow{\nabla} \times \overrightarrow{\mathbf{A}} = \overrightarrow{\mathbf{\Omega}}$, which yields the wanted result:

$$\frac{\delta\omega[\overrightarrow{\Omega}]}{\delta\overrightarrow{\mathbf{\Omega}}} \cdot \overrightarrow{\delta\mathbf{\Omega}} = \int_0^\beta d\tau \left[\overrightarrow{\mathbf{\Omega}} \cdot \left(\dot{\overrightarrow{\mathbf{\Omega}}} \times \overrightarrow{\delta\mathbf{\Omega}}\right)\right] = \int_0^\beta d\tau \left[\left(\overrightarrow{\mathbf{\Omega}} \times \dot{\overrightarrow{\mathbf{\Omega}}}\right) \cdot \overrightarrow{\delta\mathbf{\Omega}}\right]$$

[This page was intentionally left blank]

D. Appendix

D.1. Calculation of the Overlaps between the AKLT States

In this Appendix, we will obtain the overlaps and norms of the AKLT ground-states using the diagrammatic techniques developed in the main text. Starting from the even chain case, we wish to calculate the inner product $\left(\Omega^{(N)}{}_{\alpha}^{\beta}, \Omega^{(N)}{}_{\gamma}^{\delta}\right)$, which is seen to be a sum of one diagram with have two paths running around the whole diagram without breaks /we call it unbroken diagram in the [Figure D.1]) and also a whole bunch of broken diagrams which can contain a number between 0 to $N-1$ loops inside.

The unbroken contribution is just $\delta_{\alpha}^{\beta}\delta_{\gamma}^{\delta}$, while each different broken diagram contributes with $2^{\#loops}\delta_{\alpha\gamma}\delta^{\beta\delta}$. The only thing that one has to do now is count how many diagrams there are for each possible number of loops, and that is easily seen to be $\binom{N}{\#loops+1}$. Hence, we have the expression:

$$\left(\Omega^{(N)}{}_{\alpha}^{\beta}, \Omega^{(N)}{}_{\gamma}^{\delta}\right) = \delta_{\alpha}^{\beta}\delta_{\gamma}^{\delta} + \delta_{\alpha\gamma}\delta^{\beta\delta}\sum_{k=0}^{N-1}\binom{N}{k+1}2^{k} = \delta_{\alpha}^{\beta}\delta_{\gamma}^{\delta} + \frac{1}{2}\left[3^{N}-1\right]\delta_{\alpha\gamma}\delta^{\beta\delta} \tag{D.1}$$

For the case when N is odd, the contributions of the broken diagrams are unchanged, and only the unbroken one is now equal to $\delta_{\alpha\delta}\delta_{\beta\gamma}$, which yields:

$$\left(\Omega^{(N)}{}_{\alpha\beta}, \Omega^{(N)}{}_{\gamma\delta}\right) = \delta_{\alpha\delta}\delta_{\beta\gamma} + \frac{1}{2}\left[3^{N}-1\right]\delta_{\alpha\gamma}\delta^{\beta\delta} \tag{D.2}$$

□

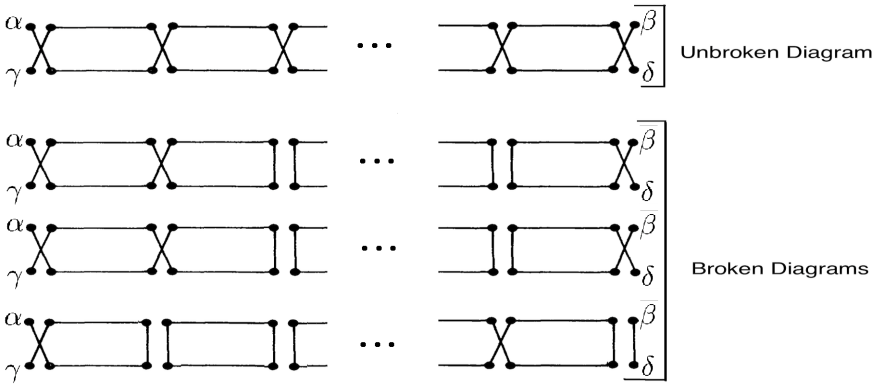


Figure D.1.: Diagrams involved in the calculation of $\left(\Omega^{(N)}{}_{\alpha}^{\beta}, \Omega^{(N)}{}_{\gamma}^{\delta}\right)$.

D.2. Calculation of Spin Averages and Correlations in the AKLT States

First of all, we want to calculate the average spin $\frac{\left(\Omega^{(N)}{}_{\alpha\beta}, S_0\Omega^{(N)}{}_{\alpha\beta}\right)}{\left(\Omega^{(N)}{}_{\alpha\beta}, \Omega^{(N)}{}_{\alpha\beta}\right)}$, for a chain with $2N+1$ sites, centered at 0. To do that we can use the usual diagrammatic techniques, and since we know that any diagram where the operator S_0^a is contained in a loop is automatically null[1], we may sum only over those diagram in which the i-th site is connected to one of the tips. There are three different groups of such diagrams, as shown in the [Figure D.2].

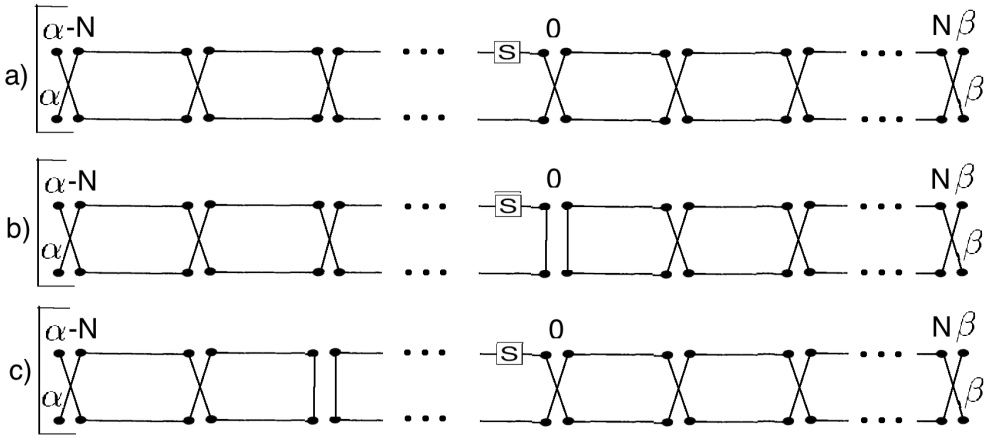


Figure D.2.: The only diagrams that contribute to $\left(\Omega^{(N)}{}_{\alpha\beta}, S_0\Omega^{(N)}{}_{\alpha\beta}\right)$. a) The unique unbroken diagram; b) The set of diagrams unbroken at the left of the operator insertion; c) The set of diagrams unbroken at the right of the operator insertion. Identical diagrams appear for the case when the insertion is at the right side of the site 0.

The first of these diagrams is unique and contributes with $-\frac{1}{2}\sigma^a_{\alpha\beta}$. The second type amounts to a contribution of $-\frac{1}{2}\sigma^a_{\beta\beta}\times\sum_{l=1}^{N+1}\binom{N+1}{l}2^{l-1}$ and the third type contributes with $-\frac{1}{2}\sigma^a_{\alpha\alpha}\times\sum_{l=1}^{N}\binom{N}{l}2^{l-1}$. For the other insertion of the operator S_0^a, we have similar contributions. In the end, we get:

$$\frac{\left(\Omega^{(N)}{}_{\alpha\beta}, S_0^a\Omega^{(N)}{}_{\alpha\beta}\right)}{\left(\Omega^{(N)}{}_{\alpha\beta}, \Omega^{(N)}{}_{\alpha\beta}\right)} = -\frac{2}{3^{2N+1}-1}\left[\sigma^a_{\alpha\beta}+\frac{1}{4}\left[\sigma^a_{\alpha\alpha}+\sigma^a_{\beta\beta}\right]\left[3^{N+1}+3^N-2\right]\right] \tag{D.3}$$

The last formula is correct and simple, but it is specific of the site in question, i.e. $i=0$. However, one is usually interested in taking the limit when $N\to\infty$, where the system has lattice translation symmetry. Thus we have, in that limit:

$$\frac{\left(\Omega^{(\infty)}{}_{\alpha\beta}, S_i^a\Omega^{(\infty)}{}_{\alpha\beta}\right)}{\left(\Omega^{(\infty)}{}_{\alpha\beta}, \Omega^{(\infty)}{}_{\alpha\beta}\right)} = \lim_{N\to\infty}\left\{\frac{\left(\Omega^{(N)}{}_{\alpha\beta}, S_0^a\Omega^{(N)}{}_{\alpha\beta}\right)}{\left(\Omega^{(N)}{}_{\alpha\beta}, \Omega^{(N)}{}_{\alpha\beta}\right)}\right\} = 0 \tag{D.4}$$

In fact, this result is obtained directly if one does the calculation with the state $\Omega^{(N)}_{PBC}$ for any N!Another interesting quantity one wants to obtain is the two point correlation function, i.e.:

[1]Because the contribution will be proportional to $Tr\left[\sigma^a\right]=0$!

$$C^{ab}(r) \equiv \frac{\left(\Omega^{(N)}{}_{\alpha\beta}, S_0^a S_r^b \Omega^{(N)}{}_{\alpha\beta}\right)}{\left(\Omega^{(N)}{}_{\alpha\beta}, \Omega^{(N)}{}_{\alpha\beta}\right)} \tag{D.5}$$

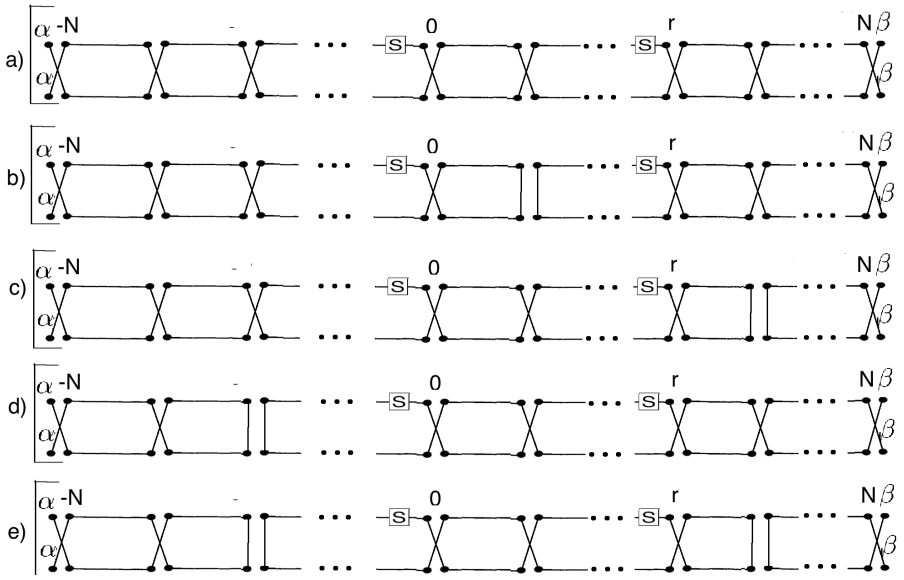


Figure D.3.: Diagrams representing the 5 types of diagrams that contribute to the calculation of $\left(\Omega^{(N)}{}_{\alpha\beta}, S_0^a S_r^b \Omega^{(N)}{}_{\alpha\beta}\right)$ using the first case of insertions from Figure 6. We have the single unbroken diagram (a), one that is broken only between the insertions (b), the ones that are broken only to the right (c) or to the left (d) of both insertions, and the ones in which both insertions are contained in a same loop (e).

This is to be done diagrammatically for all the possible insertions of the operators, as explained in the Figure 4.6 of the main text. For a start, let's consider only the first of those cases, where one knows that $\left(\Omega^{(N)}{}_{\alpha\beta}, S_0^a S_r^b \Omega^{(N)}{}_{\alpha\beta}\right)$ only receives contributions from diagrams where S_0^a and S_r^b do not belong to different loops. So we must only consider diagrams of the types shown in the Figure C.3, yielding the following contributions:

- Unbroken, contributing with:

$$\frac{1}{4}\sigma^a_{\alpha\beta}\sigma^b{}_{\alpha\beta} \quad if\ r\ is\ odd \tag{D.6}$$

$$-\frac{1}{4}\sigma^a_{\alpha\gamma}\sigma^b{}_{\gamma\beta} = -\frac{1}{4}\left[\sigma^a \cdot \sigma^b\right]_{\alpha\beta} \quad if\ r\ is\ even \tag{D.7}$$

- Broken only in between the operators,which yields:

$$\frac{1}{4}\sigma^a_{\alpha\alpha}\sigma^b{}_{\beta\beta}\sum_{l=1}^{r}\binom{r}{l}2^{l-1} = \frac{1}{8}\left[3^r-1\right]\sigma^a_{\alpha\alpha}\sigma^b{}_{\beta\beta} \quad if\ r\ is\ odd \tag{D.8}$$

$$-\frac{1}{4}\sigma^a_{\alpha\alpha}\sigma^b{}_{\beta\beta}\sum_{l=1}^{r}\binom{r}{l}2^{l-1} = -\frac{1}{8}\left[3^r-1\right]\sigma^a_{\alpha\alpha}\sigma^b{}_{\beta\beta} \quad if\ r\ is\ even \tag{D.9}$$

- Broken only at the left of both operators:

$$\frac{1}{4}\sigma^a_{\beta\beta}\sigma^b_{\beta\beta}\sum_{l=1}^{N}\binom{N}{l}2^{l-1}=\frac{1}{8}\left[3^N-1\right]\sigma^a_{\beta\beta}\sigma^b_{\beta\beta}\quad if\ r\ is\ odd \tag{D.10}$$

$$-\frac{1}{4}\sum_{\gamma}\sigma^a_{\beta\gamma}\sigma^b_{\gamma\beta}\sum_{l=1}^{N}\binom{N}{l}2^{l-1}=-\frac{1}{8}\left[3^N-1\right]\left[\sigma^a\cdot\sigma^b\right]_{\beta\beta}\quad if\ r\ is\ even \tag{D.11}$$

- Broken only at the right of both operators:

$$\frac{1}{4}\sigma^a_{\beta\beta}\sigma^b_{\beta\beta}\sum_{l=1}^{N-r+1}\binom{N-r+1}{l}2^{l-1}=\frac{1}{8}\left[3^{N-r+1}-1\right]\sigma^a_{\beta\beta}\sigma^b_{\beta\beta}\quad if\ r\ is\ odd \tag{D.12}$$

$$-\frac{1}{4}\sum_{\gamma}\sigma^a_{\beta\gamma}\sigma^b_{\gamma\beta}\sum_{l=1}^{N-r+1}\binom{N-r+1}{l}2^{l-1}=-\frac{1}{8}\left[3^{N-r+1}-1\right]\left[\sigma^a\cdot\sigma^b\right]_{\beta\beta}\quad if\ r\ is\ even \tag{D.13}$$

- Broken the left and right, while not in between both operators:

$$\frac{1}{4}Tr\left[\sigma^a\cdot\sigma^b\right]\sum_{l=2}^{2N-r+1}\binom{2N-r+1}{l}2^{l-2}=\frac{1}{8}\left[3^{2N-r+1}-3-2r-4N\right]\delta^{ab}\quad if\ r\ is\ odd \tag{D.14}$$

$$-\frac{1}{4}Tr\left[\sigma^a\cdot\sigma^b\right]\sum_{l=2}^{2N-r+1}\binom{2N-r+1}{l}2^{l-2}=-\frac{1}{8}\left[3^{2N-r+1}-3-2r-4N\right]\delta^{ab}\quad if\ r\ is\ odd \tag{D.15}$$

Now, the true value of $C^{ab}(r)$ is the sum of all 5 contributions calculated above, plus all the ones arising from the remaining 3 insertions. However, if one is interested in considering the thermodynamic limit - $N\to\infty$ - we can simply see that the only term that will contribute to the limit is the (4.104) or (4.105), because they are of the same order of magnitude as the norm of the AKLT state, i.e. 3^{2N}. Therefore the contribution of the case considered is, in that limit, equal to:

$$\sim(-1)^{r+1}\frac{1}{4}\delta^{ab}\frac{3^{2N-r+1}}{3^{2N+1}}=(-1)^{r+1}\frac{1}{4}\delta^{ab}3^{-r} \tag{D.16}$$

The relevant contributions from all the other cases in Figure 4.6 are given by (sequentially, according to Figure 4.6):

$$(-1)^{r+1}\frac{1}{4}Tr\left[\sigma^a\cdot\sigma^b\right]\sum_{l=2}^{2N-r+2}\binom{2N-r+2}{l}2^{l-2}=(-1)^{r+1}\frac{1}{8}\delta^{ab}\left[3^{2N-r+2}-5-2r-4N\right] \tag{D.17}$$

$$(-1)^{r+1}\frac{1}{4}Tr\left[\sigma^a\cdot\sigma^b\right]\sum_{l=2}^{2N-r}\binom{2N-r+2}{l}2^{l-2}=(-1)^{r+1}\frac{1}{8}\delta^{ab}\left[3^{2N-r}-1-2r-4N\right] \tag{D.18}$$

$$(-1)^{r+1}\frac{1}{4}Tr\left[\sigma^a\cdot\sigma^b\right]\sum_{l=2}^{2N-r+1}\binom{2N-r+1}{l}2^{l-2}=(-1)^{r+1}\frac{1}{8}\left[3^{2N-r+1}-3-2r-4N\right]\delta^{ab} \tag{D.19}$$

Summing all the 4 contributions in the thermodynamic limit, we achieve the wanted result:

$$C^{ab}(r) = {}^{4}\!/_{3}(-1)^{r+1}\delta^{ab}3^{-r} \tag{D.20}$$

D.3. Calculations for the proof of Lemma 6

In this Appendix, we will calculate explicitly the overlaps and norms needed in the proof of Lemma 6. For that we will make abundant use of the overlaps between VBS states (eqs. (4.85)-(4.86)), for which we restate de results:

$$\left(\Omega^{(N)}{}_{\alpha}^{\beta}, \Omega^{(N)}{}_{\gamma}^{\delta}\right) = \delta_{\alpha}^{\beta}\delta_{\gamma}^{\delta} + \frac{1}{2}\left[3^N - 1\right]\delta_{\alpha\gamma}\delta^{\beta\delta} \; for \; N \; even$$

$$\left(\Omega^{(N)}{}_{\alpha\beta}, \Omega^{(N)}{}_{\gamma\delta}\right) = \delta_{\alpha\delta}\delta_{\beta\gamma} + \frac{1}{2}\left[3^N - 1\right]\delta_{\alpha\gamma}\delta^{\beta\delta} \; for \; N \; odd$$

And also, the basic result:

$$(\psi_{\alpha\beta}, \psi_{\gamma\delta}) = \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}$$

We start by calculating the constraint equation for the coefficients of φ, imposing normalization:

$$\begin{aligned}
(\varphi,\varphi) = \left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\nu}^{\mu\,\rho\epsilon}\left(\Omega_{\alpha\;\beta\;\delta\sigma}^{\;\beta\;\gamma}, \Omega_{\mu\;\lambda\;\rho\epsilon}^{\;\lambda\;\nu}\right) &= \left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\nu}^{\mu\,\rho\epsilon}\left(\Omega^{(n)}{}_{\alpha}^{\;\;\gamma}, \Omega^{(n)}{}_{\mu}^{\;\;\nu}\right)(\psi_{\delta\sigma}, \psi_{\rho\epsilon}) \\
&= \left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\nu}^{\mu\,\rho\epsilon}\left[\delta_{\alpha}^{\gamma}\delta_{\mu}^{\nu} + \frac{1}{2}(3^n-1)\delta_{\alpha\mu}\delta^{\gamma\nu}\right][\delta_{\delta\rho}\delta_{\sigma\epsilon} + \delta_{\delta\epsilon}\delta_{\sigma\rho}] = \\
&= \left[\left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\nu\delta\sigma}^{\mu} + \left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\nu\sigma\delta}^{\mu}\right]\left[\delta_{\alpha}^{\gamma}\delta_{\mu}^{\nu} + \frac{1}{2}(3^n-1)\delta_{\alpha\mu}\delta^{\gamma\nu}\right] = \\
= 2\left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\nu\delta\sigma}^{\mu}\left[\delta_{\alpha}^{\gamma}\delta_{\mu}^{\nu} + \frac{1}{2}(3^n-1)\delta_{\alpha\mu}\delta^{\gamma\nu}\right] &= 2\left[A_{\alpha}^{\alpha\,\delta\sigma}\right]^{*} A_{\mu\delta\sigma}^{\mu} + (3^n-1)\left[A_{\gamma}^{\alpha\,\delta\sigma}\right]^{*} A_{\alpha\;\delta\sigma}^{\gamma} = \\
&= 2\sum_{\delta\sigma}\left|\sum_{\alpha} A_{\alpha}^{\alpha\,\delta\sigma}\right|^2 + (3^n-1)\sum_{\alpha\gamma\delta\sigma}\left|A_{\gamma}^{\alpha\,\delta\sigma}\right|^2
\end{aligned}$$

Equating this last expression to 1, we get equation (4.119) of the main text:

$$2\sum_{\delta\sigma}\left|\sum_{\alpha} A_{\alpha}^{\alpha\,\delta\sigma}\right|^2 + (3^n-1)\sum_{\alpha\gamma\delta\sigma}\left|A_{\gamma}^{\alpha\,\delta\sigma}\right|^2 = 1$$

To obtain the expression (4.122) for the constraint of orthogonality between φ and the ground-state subspace for the AKLT chain, we had to calculate the following overlap:

$$\begin{aligned}\left(\Omega_{\alpha\,\beta\,\gamma\delta}^{\ \ \beta\ \ \gamma},\varphi\right) =& A_{\nu}^{\mu\,\sigma\rho}\left(\Omega_{\alpha\,\beta\,\gamma\delta}^{\ \ \beta\ \ \gamma},\Omega_{\mu\,\beta\ \ \sigma\rho}^{\ \ \beta\ \ \nu}\right) = A_{\nu}^{\mu\,\sigma\rho}\left(\Omega^{(n)}{}_{\alpha}^{\ \gamma},\Omega^{(n)}{}_{\mu}^{\ \nu}\right)(\psi_{\gamma\delta},\psi_{\sigma\rho}) = \\ =& \left[\delta_{\alpha}^{\ \gamma}\delta_{\mu}^{\ \nu}+\frac{1}{2}(3^n-1)\delta_{\alpha\mu}\delta^{\gamma\nu}\right]\left[\delta_{\gamma\sigma}\delta_{\delta\rho}+\delta_{\gamma\rho}\delta_{\delta\sigma}\right]A_{\nu}^{\mu\,\sigma\rho} = \\ =& \left[\delta_{\alpha}^{\ \gamma}\delta_{\mu}^{\ \nu}+\frac{1}{2}(3^n-1)\delta_{\alpha\mu}\delta^{\gamma\nu}\right]\left[A_{\nu\gamma\delta}^{\mu}+A_{\nu\delta\gamma}^{\mu}\right] = 2\left[\delta_{\alpha}^{\ \gamma}\delta_{\mu}^{\ \nu}+\frac{1}{2}(3^n-1)\delta_{\alpha\mu}\delta^{\gamma\nu}\right]A_{\nu\gamma\delta}^{\mu} = \\ =& 2A_{\mu\,\alpha\delta}^{\ \ \mu}+(3^n-1)A_{\alpha\,\gamma\delta}^{\ \ \gamma}\end{aligned}$$

By setting the above expression to zero, we get exactly the wanted expression:

$$2A_{\mu\,\alpha\delta}^{\ \ \mu}+(3^n-1)A_{\alpha\,\gamma\delta}^{\ \ \gamma}=0$$

Finally, we need to calculate the overlap $(\varphi, Q_{n-l+1,n+1}\varphi)$, in order to obtain the expression (4.125). That calculation goes as follows (where we assume, without loss of generality, that $l$is an even integer):

$$\begin{aligned}& D_{\beta}^{\alpha\,\gamma\sigma}A_{\nu}^{\mu\,\rho\epsilon}\left(\Omega_{\mu\,\lambda\ \ \rho\epsilon}^{\ \ \lambda\ \ \nu},\Omega_{\alpha\,\gamma\ \ \delta\sigma}^{\ \ \beta\ \ \delta}\right) = \\ =& D_{\beta}^{\alpha\,\gamma\sigma}A_{\nu}^{\mu\,\rho\epsilon}\left(\Omega^{(l)}{}_{\mu}^{\ \lambda},\Omega^{(l)}{}_{\alpha}^{\ \beta}\right)\left(\Omega^{(n-l)}{}_{\lambda}^{\ \nu},\Omega^{(n-l)}{}_{\gamma}^{\ \delta}\right)(\psi_{\rho\epsilon},\psi_{\delta\sigma}) = \\ =& \left[\delta_{\mu}^{\ \lambda}\delta_{\alpha}^{\ \beta}+\frac{1}{2}(3^l-1)\delta_{\mu\alpha}\delta^{\lambda\beta}\right]\left[\delta_{\lambda}^{\ \nu}\delta_{\gamma}^{\ \delta}+\frac{1}{2}(3^{n-l}-1)\delta_{\lambda\gamma}\delta^{\nu\delta}\right]\left[\delta_{\rho\delta}\delta_{\epsilon\sigma}+\delta_{\rho\sigma}\delta_{\epsilon\delta}\right]D_{\beta}^{\alpha\,\gamma\sigma}A_{\nu}^{\mu\,\rho\epsilon} = \\ =& 2\left[\delta_{\mu}^{\ \lambda}\delta_{\alpha}^{\ \beta}+\frac{1}{2}(3^l-1)\delta_{\mu\alpha}\delta^{\lambda\beta}\right]\left[\delta_{\lambda}^{\ \nu}\delta_{\gamma}^{\ \delta}+\frac{1}{2}(3^{n-l}-1)\delta_{\lambda\gamma}\delta^{\nu\delta}\right]D_{\beta}^{\alpha\,\gamma\sigma}A_{\nu\delta\sigma}^{\mu} = \\ =& 2\left[\delta_{\mu}^{\ \lambda}\delta_{\alpha}^{\ \beta}+\frac{1}{2}(3^l-1)\delta_{\mu\alpha}\delta^{\lambda\beta}\right]\left[D_{\beta}^{\alpha\,\delta\sigma}A_{\nu\delta\sigma}^{\mu}\delta_{\lambda}^{\ \nu}+\frac{1}{2}(3^{n-l}-1)D_{\beta\lambda}^{\alpha\ \ \sigma}A_{\ \delta\sigma}^{\mu\delta}\right] = \\ =& 2D_{\alpha}^{\alpha\,\delta\sigma}A_{\nu\delta\sigma}^{\nu}+(3^l-1)D_{\beta}^{\alpha\,\delta\sigma}A_{\alpha\,\delta\sigma}^{\beta}+(3^{n-l}-1)D_{\alpha}^{\alpha\,\mu\sigma}A_{\mu\,\delta\sigma}^{\ \ \delta}+\frac{1}{2}(3^l-1)(3^{n-l}-1)D_{\beta}^{\alpha\,\beta\sigma}A_{\alpha\,\delta\sigma}^{\ \ \delta} = \\ =& 2D_{\delta}^{\delta\,\beta\gamma}A_{\alpha\,\beta\gamma}^{\ \ \alpha}+(3^l-1)D_{\beta}^{\alpha\,\gamma\delta}A_{\alpha\,\gamma\delta}^{\ \ \beta}+(3^{n-l}-1)D_{\delta}^{\delta\,\alpha\gamma}A_{\alpha\,\beta\gamma}^{\ \ \beta}+\frac{1}{2}(3^{n-l}-1)(3^l-1)D_{\delta}^{\alpha\,\delta\gamma}A_{\alpha\,\beta\gamma}^{\ \ \beta}\end{aligned}$$

Where last step consisted only of an index renaming to get the form used in the main text.

D.4. SU(2) invariant combination of Schwinger Bosons

In this short Appendix, we will prove that the combination $\left(a_i^\dagger b_{i+1}^\dagger - a_{i+1}^\dagger b_i^\dagger\right)$ is an invariant under any rotation, which can be implemented by the unitary operator - $U(\theta,\phi)$. For that, we just need to calculate, using (4.137):

$$\begin{aligned}\tilde{a}_i^\dagger\tilde{b}_{i+1}^\dagger =& \left[e^{-i\phi/2}\cos(\theta/2)\,a_i^\dagger+e^{i\phi/2}\sin(\theta/2)\,b_i^\dagger\right]\left[-e^{-i\phi/2}\sin(\theta/2)\,a_{i+1}^\dagger+e^{i\phi/2}\cos(\theta/2)\,b_{i+1}^\dagger\right] = \\ =& \cos(\theta/2)\sin(\theta/2)\left[e^{i\phi}b_i^\dagger b_{i+1}^\dagger-e^{-i\phi}a_i^\dagger a_{i+1}^\dagger\right]+\cos^2(\theta/2)\,a_i^\dagger b_{i+1}^\dagger-\sin^2(\theta/2)\,b_i^\dagger a_{i+1}^\dagger\end{aligned}$$

$$\tilde{a}_{i+1}^{\dagger}\tilde{b}_{i}^{\dagger}=\left[e^{-i\phi/2}\cos\left(\theta/2\right)a_{i+1}^{\dagger}+e^{i\phi/2}\sin\left(\theta/2\right)b_{i+1}^{\dagger}\right]\left[-e^{-i\phi/2}\sin\left(\theta/2\right)a_{i}^{\dagger}+e^{i\phi/2}\cos\left(\theta/2\right)b_{i}^{\dagger}\right]=$$
$$=\cos\left(\theta/2\right)\sin\left(\theta/2\right)\left[e^{i\phi}b_{i}^{\dagger}b_{i+1}^{\dagger}-e^{-i\phi}a_{i}^{\dagger}a_{i+1}^{\dagger}\right]+\cos^{2}\left(\theta/2\right)a_{i+1}^{\dagger}b_{i}^{\dagger}-\sin^{2}\left(\theta/2\right)b_{i+1}^{\dagger}a_{i}^{\dagger}$$

Meaning that:

$$\tilde{a}_{i}^{\dagger}\tilde{b}_{i+1}^{\dagger}-\tilde{a}_{i+1}^{\dagger}\tilde{b}_{i}^{\dagger}=\left[\cos^{2}\left(\theta/2\right)+\sin^{2}\left(\theta/2\right)\right]\left[a_{i+1}^{\dagger}b_{i}^{\dagger}-b_{i+1}^{\dagger}a_{i}^{\dagger}\right]=a_{i+1}^{\dagger}b_{i}^{\dagger}-b_{i+1}^{\dagger}a_{i}^{\dagger}$$

Which proved the wanted result.

D.5. Calculation of the Double-Commutator for the SMA

In this Appendix, we wish to calculate the value of the double-commutator defined in (4.164):

$$\langle AKLT|\left[S_{-q}^{\alpha},\left[H_{AKLT},S_{q}^{\alpha}\right]\right]|AKLT\rangle$$

We start by noting that the following simplification can be done using the symmetries of the AKLT ground-state (namely the rotational symmetry):

$$\begin{aligned}
&\left\langle\left[S_{-q}^{\alpha},\left[H_{AKLT},S_{q}^{\alpha}\right]\right]\right\rangle=\frac{1}{N^{2}}\sum_{j}\sum_{m,n}\left\langle\left[S_{m}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{n}^{z}\right]\right]\right\rangle e^{-iqa(n-m)}=\\
&=\frac{1}{N^{2}}\sum_{j}\sum_{m,n}\left\langle\left[S_{m}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{n}^{z}\right]\right]\right\rangle\left\{\delta_{m,j}\delta_{n,j}+\delta_{m,j+1}\delta_{n,j}+\delta_{m,j}\delta_{n,j+1}+\delta_{m,j+1}\delta_{n,j+1}\right\}e^{-iqa(n-m)}=\\
&=\frac{1}{N^{2}}\sum_{j}\left\{\left\langle\left[S_{j}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{j}^{z}\right]\right]\right\rangle+\left(e^{iqa}+e^{-iqa}\right)\left\langle\left[S_{j+1}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{j}^{z}\right]\right]\right\rangle+\right.\\
&\left.+\left\langle\left[S_{j+1}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{j+1}^{z}\right]\right]\right\rangle\right\}=\\
&=\frac{2}{N^{2}}\sum_{j}\left\{\left\langle\left[S_{j}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{j}^{z}\right]\right]\right\rangle+\cos qa\left\langle\left[S_{j+1}^{z},\left[P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S_{j}^{z}\right]\right]\right\rangle\right\}=
\end{aligned}$$

Specializing for our case of interest - $P\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)=\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)+1/3\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)^{2}$, we have the following partial results:

$$\left[S_{j+1}^{z},\left[\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1},S_{j+1}^{z}\right]\right]=\left[S_{j}^{z},\left[\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1},S_{j}^{z}\right]\right]==i\left[S_{j}^{z},S_{j}^{x}S_{j+1}^{y}-S_{j}^{y}S_{j+1}^{x}\right]=-\left(S_{j}^{x}S_{j+1}^{x}+S_{j}^{y}S_{j+1}^{y}\right)$$

$$\left[S_{j}^{z},\left[\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1},S_{j+1}^{z}\right]\right]=\left[S_{j+1}^{z},\left[\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1},S_{j}^{z}\right]\right]=i\left[S_{j+1}^{z},S_{j}^{x}S_{j+1}^{y}-S_{j}^{y}S_{j+1}^{x}\right]=\left(S_{j}^{x}S_{j+1}^{x}+S_{j}^{y}S_{j+1}^{y}\right)$$

$$\begin{aligned}
\left[S_{j}^{z},\left[\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)^{2},S_{j}^{z}\right]\right]&=i\left[S_{j}^{z},\left(S_{j}^{x}S_{j+1}^{y}-S_{j}^{y}S_{j+1}^{x}\right)\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)+\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)\left(S_{j}^{x}S_{j+1}^{y}-S_{j}^{y}S_{j+1}^{x}\right)\right]=\\
&=2\left(S_{j}^{x}S_{j+1}^{y}-S_{j}^{y}S_{j+1}^{x}\right)^{2}-\left(S_{j}^{x}S_{j+1}^{x}+S_{j}^{y}S_{j+1}^{y}\right)\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)-\\
&-\left(\overrightarrow{\mathbf{S}}_{j}\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)\left(S_{j}^{x}S_{j+1}^{x}+S_{j}^{y}S_{j+1}^{y}\right)
\end{aligned}$$

$$\left[S^z_{j+1},\left[\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)^2,S^z_j\right]\right]=i\left[S^z_{j+1},\left(S^x_jS^y_{j+1}-S^y_jS^x_{j+1}\right)\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)+\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)\left(S^x_jS^y_{j+1}-S^y_jS^x_{j+1}\right)\right]=$$
$$=-2\left(S^x_jS^y_{j+1}-S^y_jS^x_{j+1}\right)^2+\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)+$$
$$+\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)$$

From the above results, we notice that $\left[S^z_j,\left[P\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S^z_j\right]\right]=-\left[S^z_{j-1},\left[P\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right),S^z_j\right]\right]$ for the AKLT case. Therefore, we can write the following result:

$$\langle AKLT|\left[S^z_{-q},\left[H_{AKLT},S^z_q\right]\right]|AKLT\rangle=-\frac{J}{N^2}\left\{\sum\langle AKLT|A_j|AKLT\rangle\right\}\left[1-\cos qa\right] \tag{D.21}$$

Where A_j is defined as:

$$A_j=2\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)+{}^2\!/_3\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)+$$
$$+{}^2\!/_3\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)-{}^4\!/_3\left(S^x_jS^y_{j+1}-S^y_jS^x_{j+1}\right)^2$$

Now, using the fact the $|AKLT\rangle$ is a global singlet state, we can establish that:

$$\sum_j\langle AKLT|\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)|AKLT\rangle=\frac{2}{3}\sum_j\langle AKLT|\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}|AKLT\rangle \tag{D.22}$$

$$\sum_j\langle AKLT|\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)|AKLT\rangle= \tag{D.23}$$
$$=\sum_j\langle AKLT|\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)\left(S^x_jS^x_{j+1}+S^y_jS^y_{j+1}\right)|AKLT\rangle= \tag{D.24}$$
$$=\frac{2}{3}\sum_j\langle AKLT|\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)^2|AKLT\rangle \tag{D.25}$$

On the other hand, one also knows that (from the energy of the AKLT ground-state):

$$\frac{1}{3}\sum_j\langle AKLT|\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)^2|AKLT\rangle=-\sum_j\langle AKLT|\left(\overrightarrow{\mathbf{S}}_j\cdot\overrightarrow{\mathbf{S}}_{j+1}\right)|AKLT\rangle-\frac{2N}{3} \tag{D.26}$$

Using all of the above results, we get:

$$
\begin{aligned}
&\sum_j \langle AKLT|\, A_j \,|AKLT\rangle = \\
&= \sum_j \left\{ \frac{4}{3} \left\langle \overrightarrow{\mathbf{S}}_j \cdot \overrightarrow{\mathbf{S}}_{j+1} \right\rangle + \frac{8}{3} \left\langle \frac{1}{3} \left(\overrightarrow{\mathbf{S}}_j \cdot \overrightarrow{\mathbf{S}}_{j+1} \right)^2 \right\rangle - \frac{4}{3} \left\langle \left(S_j^x S_{j+1}^y - S_j^y S_{j+1}^x \right)^2 \right\rangle \right\} = \\
&= -\frac{4N}{3} \left\langle \overrightarrow{\mathbf{S}}_0 \cdot \overrightarrow{\mathbf{S}}_1 \right\rangle - \frac{16N}{9} - \frac{4}{3} \sum_j \left\langle \left(S_j^x S_{j+1}^y - S_j^y S_{j+1}^x \right)^2 \right\rangle = \\
&= -\frac{4}{3} \sum_j \left\langle \left(S_j^x S_{j+1}^y - S_j^y S_{j+1}^x \right)^2 \right\rangle
\end{aligned}
$$

Which yields the expression (4.164).

[This page was intentionally left blank]

Bibliography

[1] T. Holstein, H. Primakoff, 'Field Dependence of the Intrinsic Domain Magnetization of a Ferromagnet', Phys. Rev. 58 (1940)

[2] P. W. Anderson, 'An Approximate Quantum Theory of the Antiferromagnetic Ground State', Phys. Rev. 86, 694 (1952)

[3] R. Kubo, 'The Spin-Wave Theory of Antiferromagnetics', Phys. Rev. 87, 568 (1952)

[4] N. D. Mermin, H. Wagner, 'Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models', Phys. Rev. Lett. 17-22 (1966)

[5] P. W. Anderson, 'Basic Notions in Condensed Matter Physics', 1984

[6] I. Affleck, 'Quantum Spin Chains and the Haldane Gap', J. Phys.: Condens. Matter 1 3047-3072 (1989)

[7] A. Auerbach, 'Interacting Electrons and Quantum Magnetism', Springer-Verlag (1994)

[8] C. Kittel, 'Quantum Theory of Solids', 2nd Ed., John Wiley & Sons (1987)

[9] E. Lieb, T. Schultz, D. Mattis, 'Two Soluble Models of an Antiferromagnetic Chain', Ann. Phys. 16 407-466 (1961)

[10] C. Cohen-Tannoudji, B. Diu, F. Laloé, 'Quantum Mechanics', Volume 1 Wiley-VCH (1977)

[11] H. Goldstein, C. Poole, J. Safko, 'Classical Mechanics', 3rd Edition, Addison Wesley (2000)

[12] J. M. Radcliffe, 'Some Properties of Coherent Spin States', J. Phys. A: Gen Phys. 4, 313-323 (1971)

[13] P. W. Atkins, J. C. Dobson, 'Angular Momentum Coherent States', Proc. Roy. Soc. Lond. A. 321, 321-340 (1971)

[14] S. D. Deshpande, R. B. Pode, 'Matrix Representation of Vectors and Operators in Non-orthogonal Basis Vectors', Am. J. Phys., 56 (4) (1988)

[15] J. Kutzner, 'Eine Phasenraumdarstellung für Spinsysteme', Z. Physik 259, 177-188 (1973)

[16] J. Kutzner, 'On the Phase Space Representation for Spin Systems', Phys. Lett. A 41, 5 (1972)

[17] J. R. Klauder, B. Skagerstam, 'Coherent States - Applications in Physics and Mathematical Physics', World Scientific Publishing Co. Pte. Ltd. (1985)

[18] E. Lieb, 'The Classical Limit of Quantum Spin Systems', Commun. Math. Phys. 31, 327-340 (1973)

[19] J. Schwinger, 'Quantum Theory of Angular Momentum', Academic Press (1965)

[20] J. R. Klauder, 'Path Integrals and Stationary-Phase Approximations', Phys. Rev. D 19-8 2349 (1979)

[21] J. R. Klauder, in 'Path Integrals', Proceedings of the NATO Advanced Summer Institute, ed. by G.J. Papadopoulos and J. T. Devreese (1978)

[22] M. Peskin and D. Schroeder, 'An Introduction to Quantum Field Theory', Perseus Books Pub. (1995)

[23] F. D. M. Haldane, 'Continuum Dynamics of the 1-D Heisenberg Antiferromagnet: Identification with the O(3) Nonlinear Sigma Model', Phys. Lett. 93A 9 (1983)

[24] F. D. M. Haldane, 'Nonlinear Field Theory of Large-Spin Heisenberg Antiferromagnet: Semiclassically Quantized Solitons of the One-Dimensional Easy-Axis Néel State', Phys. Rev. Lett. 50 15 (1983)

[25] A. M Polyakov, 'Gauge Fields and Strings', Harwood Ed. (1987)

[26] A. M. Polyakov, 'Interaction of Goldstone Particles in Two-Dimensions. Applications to Ferromagnets and Massive Yang-Mills Fields', Phys. Rev. B 59, 76 (1975)

[27] I. Affleck, E. Lieb, 'A Proof of Part of Haldane's Conjecture on Spin Chains', Lett. Math. Phys. 12 57-69 (1986)

[28] C. K. Majumdar, D. K. Ghosh, "On Next-Nearest-Neighbor Interaction in the Linear Chain. I", Journ. Math. Phys 10 8 (1969)

[29] C. K. Majumdar, D. K. Ghosh, "On Next-Nearest-Neighbor Interaction in the Linear Chain. II", Journ. Math. Phys 10 8 (1969)

[30] C. K. Majumdar, "Antiferromagnetic Model with Known Ground State", Journ. Phys C: Solid State Phys. (1970)

[31] I. Affleck, T. Kennedy, E. Lieb, H. Tasaki, "Rigorous Results on Valence-Bond Ground States in Antiferromagnets", Phys. Rev. Lett. 59 7 (1987)

[32] I. Affleck, T. Kennedy, E. Lieb, H. Tasaki, "Valence-Bond Ground States in Isotropic Quantum Antiferromagnets", Commun. Math. Phys. 115 (1988)

[33] D. P. Arovas, A. Auerbach, F. D. M. Haldane, "Extended Heisenberg Models of Antiferromagnetism: Analogies to the FQH Effect", Phys. Rev. Lett. 60 6 (1988)

[34] D. P. Arovas, S. M. Girvin, 'Exact Questions to Some Interesting Answers in Manybody Physics', in 'Recent Progress in Manybody Physics, Vol 3' (1992)

[35] N. Schuch, 'Condensed Matter Applications of Entanglement Theory', arXiv:1306.5551v1 (2013)

[36] X-G Wen, 'Quantum Information Meets Quantum Matter', arXiv:1508.02595v3 (2016)

[37] W. Marshall, 'Antiferromagnetism', Proc. R. Soc. London Ser. A 232, 48 (1955)

[38] J. des Cloizeaux, J. J. Pearson, 'Spin-Wave Spectrum of the Antiferromagnetic Linear Chain', Phys. Rev. 128, 2131 (1962)

[39] J.M. Nunes da Silva, 'Renormalized Vibrations of a Loaded Spring' Am. J. Phys. 62, 493 (1994)